A comparative lipidomics platform for chemotaxonomic analysis of mycobacterium tuberculosis

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Supplemental Information

A Comparative Lipidomics Platform for Chemotaxonomic Analysis of *Mycobacterium tuberculosis*

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Inventory of Supplemental Information

Figure S1 is the *MycoMass* database whose content is summarized in Figure 1.

Figure S2 presents the previous lipidomic generation to be compared to the new generation shown in Figure 2.

Figure S3 contains additional information concerning lipid standard dose responses and detection limits, further illustrating the platform validation shown in Figure 3.

Figure S4 is a list of XCMS-extracted features from *M. tuberculosis* positive and negative ion-mode datasets and their putative annotation generated using the R script as mentioned in Figure 4A. The second part of figure S4 compiles all the collisional MS data which allowed, with other criteria, mapping *M. tuberculosis* lipid classes showed in Figure 4B and C.

Figure S5 is *MycoMap* database*;* a fine alkylforms mapping for 25 lipid classes, only 2 lipid class examples being shown in Figure 5.

Figure S6 presents PDIM MS signal *in vitro* and *in vivo* and additional experiments replicating the results presented in Figure 5.

Figure S7 provides a detailed report of all PGL features highlighted as being *M. tuberculosis* Beijing HN878 specific in the chemotaxonomic experiment presented in Figure 6C and presents the PGL MS signal detected for *M. tuberculosis* Beijing HN878 strain.

Supplemental Experimental Procedures

SUPPLEMENTAL INFORMATION

SUPPLEMENTAL FIGURES AND LEGENDS

Attached spreadsheet

Figure S1, related to Figure 1. The *MycoMass* database. The *MycoMass* database cataloged mycobacterial lipids described in the Pubmed literature sorted by lipid category, main class, subclass, and family. Alkyforms number refers to the total number of molecular species that differ by the number or nature of fatty acyl or polyketide lipid. An identification number (Number) is assigned to each molecule entry as well as a lipid class affiliation, abbreviated name, subclass affiliation, family affiliation, the total carbon number of the combined acyl units and backbone (Alkyl length), the number of unsaturations in the acyl units (Unsaturation), the formula (Formula) of the neutral mass and the calculated *m/z* of the neutral species (M) and common positively and negatively charged adducts. The database is designed as a resource for interpreting unknown compounds of known mass, so represents composite database covering many medically important mycobacteria. Therefore, the number of listed alkylforms exceeds the number of known named lipids in any one bacterial preparation. Monoglycosylated, triglycosylated phenolic glycolipids are composed of a phenolphthiocerol (A and A'), phenolphthiodiolone (B) or phenolphthiotriol (phthiotriol) or acyl phenolphthiotriol cores (C16 phthiotriol). The phthiocerol dimycocerosates present the same structural variation of their phthiocerol core. B1, B2 and B3 phenolic glycolipids are additional glycoforms described as low abundance, differing from the major phenolic glycolipids by their glycosylaton. Mycolic acids families (alpha, alpha', carboxy, epoxy, keto, methoxy and w1-carboxy) are defined based on functional groups on the meromycolic chain. The peptide core of mycobactins or carboxymycobactins differs by the presence of a serine, an α-methyl serine or a threonine and by the structure of the butyric acid that varies in methyl branchements.

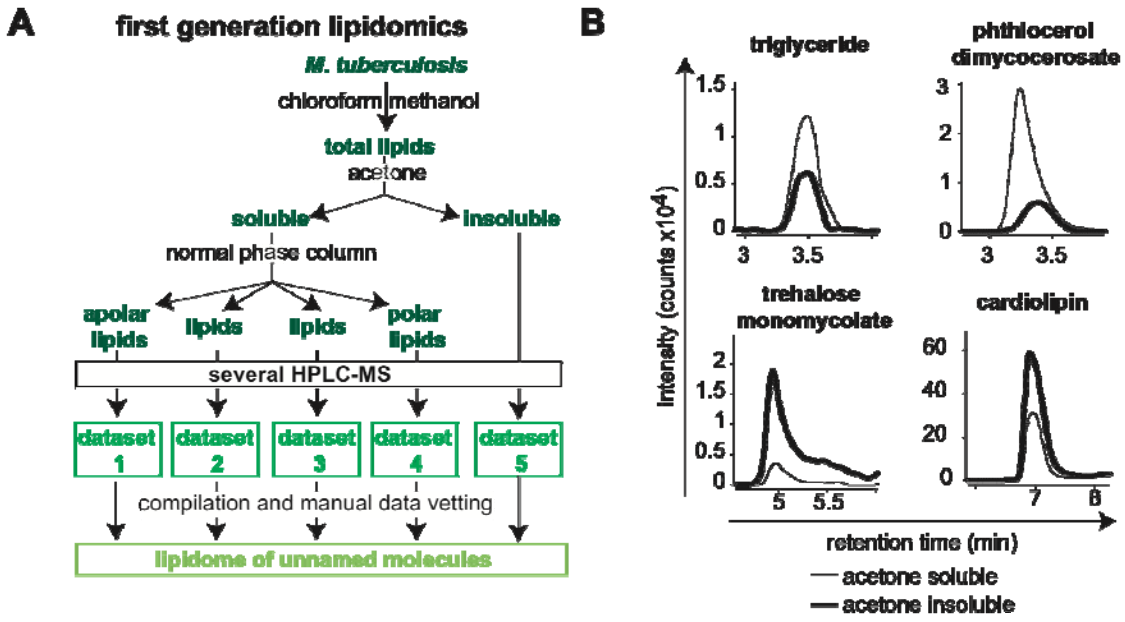


Figure S2, related to Figure 2. First generation lipidomic method. (**A**) Semi-quantitative systems extensively separate lipidic extracts by fluid-phase precipitation and normal phase chromatography (dark green), followed by HPLC-MS (black inset) to generate 5 datasets (lime green). This system provides broad chromatographic separation and separate detection of cell-associated and secreted compounds, but requires reconciling up to 10 datasets to generate one lipidome. In contrast, the second generation lipidomic system shown **Figure 1** uses a single HPLC-MS method for the direct analysis of the total lipid extract. Individual ions were confirmed by manual inspection and compiled (bright green). **(B**) After precipitation in cold acetone, all soluble (thin line) and insoluble (thick line) lipids were separately analyzed as shown in ion chromatograms extracted at the mass corresponding to the indicated lipid species, showing that many lipids partitioned into both phases of the acetone precipitation.

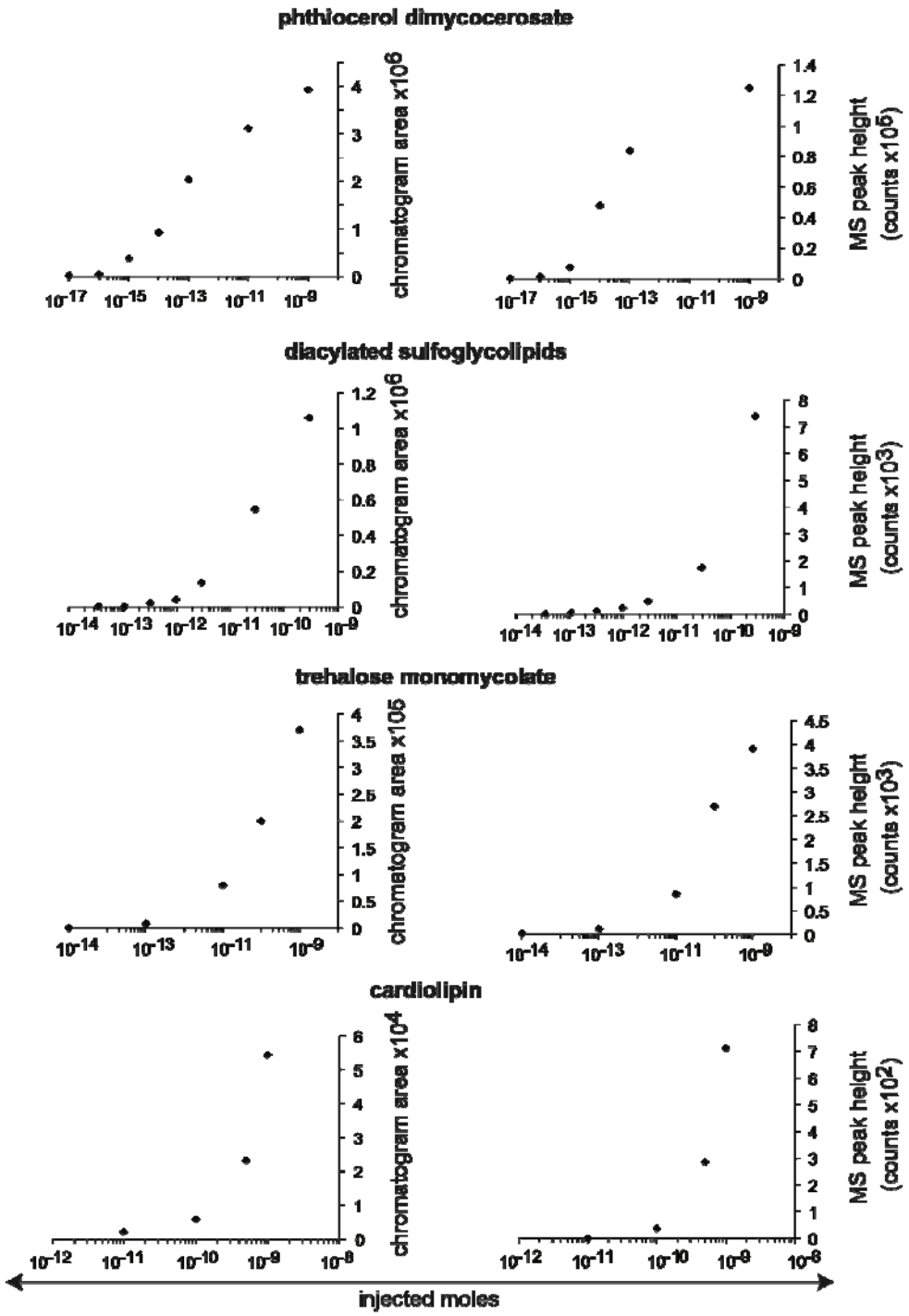


Figure S3, related to Figure 3. Lipid standards dose response and limit of detection. Standards of phthiocerol dimycocerosate (synthetic), diacylated sulfoglycolipids (purified), trehalose dimycolate (purified) and cardiolipin (Sigma) were resuspended at different concentrations and analyzed (20μl injected) as shown in area under the respective ion chromatogram (left) and mass spectral peaks height of the respective ions (right).

Figure S4, related to Figure 4. Annotations of features and confirmation by collisional MS experiments. Features (RT, *m/z* pairs) detected from replicate HPLC-MS analysis of *M. tuberculosis* H37Rv lipidic extracts were extracted using XCMS algorithm in R. The list of features was submitted to automated annotation using an in-house developed R script and *MycoMass* database with a mass tolerance of 10 ppm. Annotations were given to 625 out of 6419 total features detected in positive-ion mode (top) and to 366 out of 5240 total features detected in negative-ion mode (bottom), listed here by lipid group and RT and reporting features median *m/z* and median RT across samples. Next, to confirm annotations and map the key *M. tuberculosis* H37Rv lipid classes among detected features, one lead feature of an annotated lipid family was collided with 30-70V-collision energy in positive- and/or negative-ion mode. Subheadings indicate the studied lipid class and *m/z* of collided precursor ions. MS/MS spectra are presented with the alkylform fragmentation pattern and calculated fragments *m/z*. All fragments are protonated or deprotonated ions in positive- or negative-ion mode, respectively.

Positive-ion mode *M. tuberculosis H37Rv* dataset: 624 annotated features, 5795 features remain unannotated, 6419 features total		
Median *m/z*	Median RT(minute)	Annotation(10ppm)
1278.3501	3.7	alpha mycolic acids(88:0, 1 or 2)H+
1300.3247	3.6	alpha mycolic acids(88:0, 1 or 2)Na+
1314.336	3.6	alpha mycolic acids(89:1 or 2)Na+
1328.3596	3.6	alpha mycolic acids(90:1 or 2)Na+
1342.3735	3.6	alpha mycolic acids(91:1)Na+
1227.2629	3.6	keto mycolic acids(82:0 or 1)NH4+
1255.2856	3.6	keto mycolic acids(84:0 or 1)NH4+
1297.333	3.7	keto mycolic acids(87:0 or 1)NH4+
1226.2667	3.6	methoxy mycolic acids(83:0 or 1)H+
1254.291	3.6	methoxy mycolic acids (85:0 or 1)H+
1282.3271	3.6	methoxy mycolic acids(87:0 or 1)H+
1296.3589	3.7	methoxy mycolic acids (88:0 or 1)H+
1332.3559	3.6	methoxy mycolic acids(89:0 or 1)Na+
1315.3446	3.6	phthiocerol dimycocerosates(PDIM A and A')(54:0)NH4+ phthiotriol dimycocerosates(54:0)NH4+
1329.364	3.6	phthiocerol dimycocerosates(PDIM A and A')(54:0)NH4+ phthiotriol dimycocerosates(56:0)NH4+
1343.3844	3.6	phthiocerol dimycocerosates(PDIM A and A')(56:0)NH4+ phthiocerol dimycocerosates(PDIM A and A')(54:0)NH4+ phthiotriol dimycocerosates(57:0)NH4+
1357.3984	3.6	phthiocerol dimycocerosates(PDIM A and A')(57:0)NH4+ phthiocerol dimycocerosates(PDIM A and A')(56:0)NH4+ phthiocerol dimycocerosates(PDIM A and A')(54:0)NH4+ phthiotriol dimycocerosates(57:0)NH4+
1371.4137	3.6	phthiocerol dimycocerosates(PDIM A and A')(58:0)NH4+ phthiocerol dimycocerosates(PDIM A and A')(56:0)NH4+ phthiocerol dimycocerosates(PDIM A and A')(57:0)NH4+ phthiotriol dimycocerosates(59:0)NH4+
1385.4331	3.6	phthiocerol dimycocerosates(PDIMA and A')(59:0)NH4+ phthiocerol dimycocerosates(PDIMA and A')(57:0)NH4+ phthiocerol dimycocerosates(PDIMA and A')(58:0)NH4+ phthiocerol dimycocerosates(PDIMA and A')(56:0)NH4+ phthiotriol dimycocerosates(57:0)NH4+
1399.4457	3.6	phthiocerol dimycocerosates(PDIMA and A')(60:0)NH4+ phthiocerol dimycocerosates(PDIMA and A')(58:0)NH4+ phthiocerol dimycocerosates(PDIMA and A')(59:0)NH4+ phthiocerol dimycocerosates(PDIMA and A')(57:0)NH4+ phthiotriol dimycocerosates(61:0)NH4+
1413.4644	3.6	phthiocerol dimycocerosates(PDIM A and A')(61:0)NH4+ phthiocerol dimycocerosates(PDIM A and A')(59:0)NH4+ phthiocerol dimycocerosates(PDIM A and A')(60:0)NH4+ phthiocerol dimycocerosates(PDIM A and A')(58:0)NH4+ phthiotriol dimycocerosates(59:0)NH4+
1427.4694	3.6	phthiocerol dimycocerosates(PDIM A and A')(62:0)NH4+ phthiocerol dimycocerosates(PDIM A and A')(60:0)NH4+ phthiocerol dimycocerosates(PDIM A and A')(61:0)NH4+ phthiocerol dimycocerosates(PDIM A and A')(59:0)NH4+ phthiotriol dimycocerosates(63:0)NH4+

		phthiocerol dimycocerosates(PDIM A and A')(63:0)NH4+ phthiocerol dimycocerosates(PDIM A and A')(61:0)NH4+
1441.4885	3.6	phthiocerol dimycocerosates(PDIM A and A')(62:0)NH4+phthiocerol dimycocerosates(PDIM A and A')(60:0)NH4+ phthiotriol dimycocerosates(61:0)NH4+
		phthiocerol dimycocerosates(PDIM A and A')(64:0)NH4+ phthiocerol dimycocerosates(PDIM A and A')(62:0)NH4+
1455.5088	3.6	phthiocerol dimycocerosates(PDIM A and A')(63:0)NH4+ phthiocerol dimycocerosates(PDIM A and A')(61:0)NH4+ phthiotriol dimycocerosates(65:0)NH4+
		phthiocerol dimycocerosates(PDIM A and A')(65:0)NH4+ phthiocerol dimycocerosates(PDIM A and A')(63:0)NH4+
1469.5202	3.6	phthiocerol dimycocerosates(PDIM A and A')(64:0)NH4+ phthiocerol dimycocerosates(PDIM A and A')(62:0)NH4+ phthiotriol dimycocerosates(63:0)NH4+
1439.4848	3.6	phthiodolone dimycocerosate(PDIM B)(63:0)NH4+ phthiodolone dimycocerosate(PDIM B)(61:0)NH4+
1453.4885	3.6	phthiodolone dimycocerosate(PDIM B)(64:0)NH4+ phthiodolone dimycocerosate(PDIM B)(62:0)NH4+
1284.2997	3.6	phthiotriol dimycocerosates(54:0)H+
1301.3314	3.6	phthiotriol dimycocerosates(54:0)NH4+
1257.2676	3.6	glycerol monomycolate alpha(80:0, 1 or 2)NH4+
1285.3026	3.6	glycerol monomycolate alpha(82:0, 1 or 2)NH4+
1299.3214	3.6	glycerol monomycolate alpha(83:1 or 2)NH4+
1313.3353	3.6	glycerol monomycolate alpha(84:0, 1 or 2)NH4+ phthiodolone dimycocerosate(PDIM B)(54:0)NH4+
1327.3546	3.6	glycerol monomycolate alpha(85:1 or 2)NH4+ phthiodolone dimycocerosate(PDIM B)(55:0)NH4+
1341.369	3.6	glycerol monomycolate alpha(86:0, 1 or 2)NH4+ phthiocerol dimycocerosatesB(56:0)NH4+ phthiodolone dimycocerosate(PDIM B)(54:0)NH4+
1355.3817	3.6	glycerol monomycolate alpha(87:1 or 2)NH4+ phthiodolone dimycocerosate(PDIM B)(57:0)NH4+
1352.3701	3.7	glycerol monomycolate alpha(88:0, 1 or 2)H+ phthiodolone dimycocerosate(PDIM B)(58:0)H+ phthiodolone dimycocerosate(PDIM B)(56:0)H+
1369.4014	3.6	glycerol monomycolate alpha(88:0, 1 or 2)NH4+ phthiodolone dimycocerosate(PDIM B)(58:0)NH4+ phthiodolone dimycocerosate(PDIM B)(56:0)NH4+
1383.4137	3.6	glycerol monomycolate alpha(89:1 or 2)NH4+ phthiodolone dimycocerosate(PDIM B)(59:0)NH4+ phthiodolone dimycocerosate(PDIM B)(57:0)NH4+
1397.4326	3.6	glycerol monomycolate alpha(90:1 or 2)NH4+ phthiodolone dimycocerosate(PDIM B)(60:0)NH4+ phthiodolone dimycocerosate(PDIM B)(58:0)NH4+
1411.4479	3.6	glycerol monomycolate alpha(91:1)NH4+ phthiodolone dimycocerosate(PDIM B)(61:0)NH4+ phthiodolone dimycocerosate(PDIM B)(59:0)NH4+
1272.2816	3.6	glycerol monomycolate methoxy(81:0 or 1)H+ alpha mycolic acids(86:0, 1 or 2)Na+
1303.3274	3.6	glycerol monomycolate methoxy(82:0 or 1)NH4+
1317.3437	3.6	glycerol monomycolate methoxy(83:0 or 1)NH4+
1429.4705	3.7	glycerol monomycolate methoxy(91:0)NH4+
796.73642	3.7	triacylglycerols(46:0)NH4+
794.72358	3.7	triacylglycerols(46:1)NH4+
824.76672	3.7	triacylglycerols(48:0)NH4+
822.75251	3.7	triacylglycerols(48:1)NH4+
852.79817	3.7	triacylglycerols(50:0)NH4+
850.78412	3.7	triacylglycerols(50:1)NH4+
848.76915	3.7	triacylglycerols(50:2)NH4+
846.75471	3.7	triacylglycerols(50:3)NH4+
866.81232	3.7	triacylglycerols(51:0)NH4+
880.82851	3.7	triacylglycerols(52:0)NH4+
878.81442	3.7	triacylglycerols(52:1)NH4+
876.80032	3.7	triacylglycerols(52:2)NH4+
874.78405	3.7	triacylglycerols(52:3)NH4+
892.82674	3.7	triacylglycerols(53:1)NH4+
906.84582	3.7	triacylglycerols(54:1)NH4+
902.81457	3.7	triacylglycerols(54:3)NH4+
936.88889	3.7	triacylglycerols(56:0)NH4+
934.87998	3.7	triacylglycerols(56:1)NH4+
964.9291	3.6	triacylglycerols(58:0)NH4+
962.91125	3.7	triacylglycerols(58:1)NH4+
960.8889	3.7	triacylglycerols(58:2)NH4+
992.95509	3.7	triacylglycerols(60:0)NH4+
990.93948	3.7	triacylglycerols(60:1)NH4+
988.92431	3.7	triacylglycerols(60:2)NH4+
1006.9679	3.7	triacylglycerols(61:0)NH4+
1245.2468	3.6	triacylglycerols(78:0)NH4+ glycerol monomycolate keto(78:0 or 1)NH4+
555.53106	3.8	monoacylglycerols(32:0)H+
577.51879	3.8	monoacylglycerols(32:0)Na+
785.62339	3.8	menaquinones(45:9)H+

853.68619	3.8	menaquinones(50:10)H+
787.63169	3.8	menaquinones(45:8)H+
717.56005	3.8	menaquinones(40:8)H+
804.66397	3.8	menaquinones(45:8)NH4+
736.6028	3.9	menaquinones(40:7)NH4+
558.50877	3.8	diacylglycerols(30:0)NH4+
556.48964	4.1	diacylglycerols(30:1)NH4+
572.52292	3.9	diacylglycerols(31:0)NH4+
569.51305	3.9	diacylglycerols(32:0)H+
586.53953	3.8	diacylglycerols(32:0)NH4+
584.52424	3.9	diacylglycerols(32:1)NH4+
600.55537	3.8	diacylglycerols(33:0)NH4+
598.54203	3.8	diacylglycerols(33:1)NH4+
597.54329	3.8	diacylglycerols(34:0)H+
614.57022	3.8	diacylglycerols(34:0)NH4+
595.53192	3.9	diacylglycerols(34:1)H+
612.55603	3.9	diacylglycerols(34:1)NH4+
610.54083	3.9	diacylglycerols(34:2)NH4+
628.58722	3.8	diacylglycerols(36:0)NH4+
626.57133	3.9	diacylglycerols(35:1)NH4+
642.60154	3.8	diacylglycerols(36:0)NH4+
640.58712	3.9	diacylglycerols(36:1)NH4+
1210.1002	3.9	glucose monomycolate alpha(70:0 or 2)Na+
1224.1121	3.9	glucose monomycolate alpha(71:1)Na+
1209.0927	3.9	glucose monomycolate carboxy(68:1)NH4+
1318.2686	4.2	monomeromycolyl diacylglycerols(85:2)H+
1346.2955	4.2	monomeromycolyl diacylglycerols(87:2)H+
1405.3473	4.2	glucose monomycolate methoxy(83:0 or 1)NH4+
1433.3772	4.2	glucose monomycolate methoxy(85:0 or 1)NH4+
331.28177	4.8	monoacylglycerols(16:0)H+
353.26537	4.9	monoacylglycerols(16:0)Na+
348.3104	4.8	monoacylglycerols(16:0)NH4+
379.28168	4.9	monoacylglycerols(18:1)Na+
374.3242	4.8	monoacylglycerols(18:1)NH4+
341.30946	4.8	leprosol(15:3)H+
530.40027	4.9	menaquinones(25:5)NH4+
279.22937	5.0	mycosanoic acids(16:0)Na+ straight chain fatty acids(16:0)Na+
293.24385	4.9	mycosanoic acids(17:0)Na+ branched fatty acids(17:0)Na+
845.67405	5.6	monodeoxymycobactins(18:0)NH4+
859.68929	5.9	monodeoxymycobactins(19:0)NH4+
831.65513	6.0	monodeoxymycobactins(17:0)NH4+
868.58097	6.2	monodeoxymycobactins(21:1)H+
870.58981	6.2	monodeoxymycobactins(21:0)H+
857.61705	6.6	dideoxymycobactins(20:0)NH4+
855.60001	6.7	dideoxymycobactins(20:1)NH4+
869.60453	6.6	dideoxymycobactins(21:1)NH4+
884.63381	5.8	diglycosylated diacylglycerol(30:0)NH4+
889.57717	5.8	diglycosylated diacylglycerol(30:0)Na+
883.63556	6.0	diglycosylated diacylglycerol(31:0)H+
867.59719	6.5	diglycosylated diacylglycerol(30:0)H+
928.6927	6.6	diglycosylated diacylglycerol(33:0)NH4+
719.35694	6.4	carboxymycobactinsmonodeoxy(7:1)NH4+
733.37223	6.2	monodeoxycarboxymycobactins(8:1)NH4+
1656.4534	6.2	trehalose monomycolate methoxy(89:0 or 1)Na+
1642.4369	6.2	trehalose monomycolate methoxy(88:0 or 1)Na+
1651.4966	6.2	trehalose monomycolate methoxy(89:0 or 1)NH4+
1678.5275	6.2	trehalose monomycolate methoxy(91:0)NH4+
1614.4082	6.2	trehalose monomycolate methoxy(86:0 or 1)Na+
1635.4711	6.2	trehalose monomycolate keto(88:0 or 1)NH4+
1665.5129	6.2	trehalose monomycolate methoxy(90:0 or 1)NH4+
1637.4835	6.3	trehalose monomycolate methoxy(88:0 or 1)NH4+
1628.4228	6.3	trehalose monomycolate methoxy(87:0 or 1)Na+
1620.4526	6.3	trehalose monomycolate methoxy(86:0 or 1)H+
1606.4396	6.3	trehalose monomycolate methoxy(87:0 or 1)H+

1623.4664	6.3	trehalose monomycolate methoxy(87:0 or 1)NH4+
1592.4323	6.3	trehalose monomycolate methoxy(86:0 or 1)H+
1607.4404	6.3	trehalose monomycolate keto(86:0 or 1)NH4+
1600.3935	6.3	trehalose monomycolate methoxy(85:0 or 1)Na+
1609.4505	6.3	trehalose monomycolate methoxy(86:0 or 1)NH4+
1621.4549	6.3	trehalose monomycolate keto(87:0 or 1)NH4+
1595.4359	6.3	trehalose monomycolate methoxy(85:0 or 1)NH4+
1563.4058	6.3	trehalose monomycolate alpha(84:0, 1 or 2)NH4+
1572.3621	6.4	trehalose monomycolate methoxy(83:0 or 1)Na+
1579.4113	6.4	trehalose monomycolate keto(84:0 or 1)NH4+
1578.4092	6.4	trehalose monomycolate methoxy(85:0 or 1)H+
1535.3785	6.4	trehalose monomycolate alpha(82:0, 1 or 2)NH4+
1593.4229	6.4	trehalose monomycolate keto(85:0 or 1)NH4+
1550.3779	6.4	trehalose monomycolate methoxy(83:0 or 1)H+
1567.4056	6.4	trehalose monomycolate methoxy(83:0 or 1)NH4+
1581.417	6.4	trehalose monomycolate methoxy(84:0 or 1)NH4+
1522.3544	6.5	trehalose monomycolate methoxy(81:0 or 1)H+
1551.3804	6.5	trehalose monomycolate keto(82:0 or 1)NH4+
1539.3729	6.5	trehalose monomycolate methoxy(81:0 or 1)NH4+
1553.3844	6.5	trehalose monomycolate methoxy(82:0 or 1)NH4+
1521.3669	6.5	trehalose monomycolate alpha(81:1 or 2)NH4+
1493.3307	6.5	trehalose monomycolate alpha(79:1 or 2)NH4+
1507.3472	6.5	trehalose monomycolate alpha(80:0, 1 or 2)NH4+
1511.3481	6.5	trehalose monomycolate methoxy(79:0 or 1)NH4+
1465.3004	6.6	trehalose monomycolate alpha(77:1 or 2)NH4+
1479.3159	6.6	trehalose monomycolate alpha(78:0, 1 or 2)NH4+
1466.2951	6.6	trehalose monomycolate methoxy(77:0 or 1)H+
1456.2471	6.6	trehalose monomycolate alpha(76:0, 1 or 2)Na+
1451.284	6.6	trehalose monomycolate alpha(76:0, 1 or 2)NH4+
1484.2763	6.6	trehalose monomycolate alpha(78:0, 1 or 2)Na+
1423.2527	6.7	trehalose monomycolate alpha(74:0, 1 or 2)NH4+
990.77866	6.4	diacyltrehaloses(43:0)NH4+
976.76564	6.4	diacyltrehaloses(42:0)NH4+
1030.8105	6.4	diacyltrehaloses(46:1)NH4+
1013.7818	6.4	diacyltrehaloses(46:1)H+
953.68428	6.4	diacyltrehaloses(40:0)Na+
999.76701	6.4	diacyltrehaloses(45:1)H+
1016.7949	6.4	diacyltrehaloses(45:1)NH4+
1028.7944	6.5	diacyltrehaloses(46:2)NH4+
1002.7784	6.5	diacyltrehaloses(44:1)NH4+
1000.7672	6.5	diacyltrehaloses(44:2)NH4+
948.7328	6.5	diacyltrehaloses(40:0)NH4+
974.74694	6.5	diacyltrehaloses(42:1)NH4+
985.74808	6.5	diacyltrehaloses(44:1)H+
1014.7789	6.5	diacyltrehaloses(45:2)NH4+
988.76503	6.5	diacyltrehaloses(43:1)NH4+
972.73722	6.5	diacyltrehaloses(42:2)NH4+
971.73638	6.5	diacyltrehaloses(43:1)H+
986.74879	6.6	diacyltrehaloses(43:2)NH4+
929.69597	6.6	diacyltrehaloses(40:1)H+
960.73011	6.7	diacyltrehaloses(41:1)NH4+
934.71405	6.7	diacyltrehaloses(39:0)NH4+
889.62222	6.9	triacyltrehaloses(36:0)H+
881.42733	6.8	mycobactins(17:1)Fe3+-2H
895.44062	6.5	mycobactins(18:1)Fe3+-2H
911.46866	6.7	mycobactins(19:0)Fe3+-2H
909.45576	6.7	mycobactins(19:1)Fe3+-2H
925.48492	6.3	mycobactins(20:0)Fe3+-2H
923.47185	6.4	mycobactins(20:1)Fe3+-2H
903.61625	6.9	mycobactins(21:0)NH4+
2560.2519	6.7	tetraacylated sulfoglycolipids(144:0)NH4+
2535.2205	6.8	tetraacylated sulfoglycolipids(144:0)Na+ tetraacylated sulfoglycolipids(146:0)H+
2532.2159	6.8	tetraacylated sulfoglycolipids(142:0)NH4+
2518.2056	6.8	tetraacylated sulfoglycolipids(141:0)NH4+

2520.2075	6.8	tetraacylated sulfoglycolipids(141:0)NH4+
2534.2152	6.8	tetraacylated sulfoglycolipids(142:0)NH4+
2531.2164	6.8	tetraacylated sulfoglycolipids(144:0)Na+ tetraacylated sulfoglycolipids(143:0)H+
2490.1761	6.8	tetraacylated sulfoglycolipids(139:0)NH4+
2504.1829	6.8	tetraacylated sulfoglycolipids(140:0)NH4+
2506.192	6.8	tetraacylated sulfoglycolipids(140:0)NH4+
2493.1793	6.8	tetraacylated sulfoglycolipids(141:0)Na+ tetraacylated sulfoglycolipids(143:0)H+
2448.1308	6.8	tetraacylated sulfoglycolipids(136:0)NH4+
2476.1507	6.8	tetraacylated sulfoglycolipids(138:0)NH4+
2489.1724	6.8	tetraacylated sulfoglycolipids(141:0)Na+ tetraacylated sulfoglycolipids(140:0)H+
2491.1659	6.8	tetraacylated sulfoglycolipids(141:0)Na+
2464.145	6.8	tetraacylated sulfoglycolipids(137:0)NH4+
2477.1562	6.8	tetraacylated sulfoglycolipids(140:0)Na+
2466.1493	6.8	tetraacylated sulfoglycolipids(139:0)Na+
2475.149	6.8	tetraacylated sulfoglycolipids(141:0)Na+ tetraacylated sulfoglycolipids(139:0)H+
2462.1397	6.8	tetraacylated sulfoglycolipids(137:0)NH4+
2406.0854	6.8	tetraacylated sulfoglycolipids(133:0)NH4+
2435.1104	6.8	tetraacylated sulfoglycolipids(137:0)Na+
2451.1378	6.8	tetraacylated sulfoglycolipids(138:0)Na+ tetraacylated sulfoglycolipids(140:0)H+
2453.1265	6.9	tetraacylated sulfoglycolipids(137:0)Na+ tetraacylated sulfoglycolipids(139:0)H+
2436.1088	6.9	tetraacylated sulfoglycolipids(135:0)NH4+
2380.0572	6.9	tetraacylated sulfoglycolipids(131:0)NH4+
2434.106	6.9	tetraacylated sulfoglycolipids(135:0)NH4+
2450.1265	6.9	tetraacylated sulfoglycolipids(136:0)NH4+
2378.0502	6.9	tetraacylated sulfoglycolipids(131:0)NH4+
2352.0246	6.9	tetraacylated sulfoglycolipids(129:0)NH4+
2365.0389	6.9	tetraacylated sulfoglycolipids(132:0)Na+
2381.0561	6.9	tetraacylated sulfoglycolipids(133:0)Na+
2406.086	6.9	tetraacylated sulfoglycolipids(133:0)NH4+
2363.0298	6.9	tetraacylated sulfoglycolipids(132:0)Na+ tetraacylated sulfoglycolipids(131:0)H+
2392.0651	6.9	tetraacylated sulfoglycolipids(132:0)NH4+
2397.0573	6.9	tetraacylated sulfoglycolipids(133:0)Na+
2322.0009	6.9	tetraacylated sulfoglycolipids(127:0)NH4+ tetraacylated sulfoglycolipids(126:0)NH4+
2366.0426	6.9	tetraacylated sulfoglycolipids(130:0)NH4+
2364.025	6.9	tetraacylated sulfoglycolipids(130:0)NH4+
2335.0038	6.9	tetraacylated sulfoglycolipids(129:0)H+
2338.0057	6.9	tetraacylated sulfoglycolipids(130:0)Na+
2368.0348	6.9	tetraacylated sulfoglycolipids(131:0)Na+ tetraacylated sulfoglycolipids(133:0)H+
2361.006	6.9	tetraacylated sulfoglycolipids(131:0)H+
2338.0113	6.9	tetraacylated sulfoglycolipids(128:0)NH4+
2367.0427	6.9	tetraacylated sulfoglycolipids(132:0)Na+ tetraacylated sulfoglycolipids(134:0)H+
2295.9639	6.9	tetraacylated sulfoglycolipids(125:0)NH4+
2348.0173	6.9	tetraacylated sulfoglycolipids(130:0)H+
2373.0062	6.9	tetraacylated sulfoglycolipids(132:0)H+
2391.0555	6.9	tetraacylated sulfoglycolipids(133:0)H+
2323.9914	6.9	tetraacylated sulfoglycolipids(127:0)NH4+
2320.9874	6.9	tetraacylated sulfoglycolipids(128:0)H+
2238.9132	6.9	tetraacylated sulfoglycolipids(124:0)Na+
2356.9975	6.9	tetraacylated sulfoglycolipids(129:0)Na+ tetraacylated sulfoglycolipids(131:0)H+
2307.9769	6.9	tetraacylated sulfoglycolipids(126:0)NH4+
2350.0188	6.9	tetraacylated sulfoglycolipids(129:0)NH4+
2306.9735	6.9	tetraacylated sulfoglycolipids(127:0)H+
2309.9773	7.0	tetraacylated sulfoglycolipids(126:0)NH4+
2279.9413	7.0	tetraacylated sulfoglycolipids(124:0)NH4+
2280.9407	7.0	tetraacylated sulfoglycolipids(126:0)Na+
2324.9868	7.0	tetraacylated sulfoglycolipids(129:0)Na+ tetraacylated sulfoglycolipids(131:0)H+
2293.9551	7.0	tetraacylated sulfoglycolipids(125:0)NH4+
2292.9527	7.0	tetraacylated sulfoglycolipids(126:0)H+
2281.9515	7.0	tetraacylated sulfoglycolipids(124:0)NH4+
2278.9353	7.0	tetraacylated sulfoglycolipids(126:0)Na+ tetraacylated sulfoglycolipids(125:0)H+
2254.9169	7.0	tetraacylated sulfoglycolipids(124:0)Na+
2282.9395	7.0	tetraacylated sulfoglycolipids(126:0)Na+ tetraacylated sulfoglycolipids(128:0)H+
2267.9347	7.0	tetraacylated sulfoglycolipids(123:0)NH4+
2251.91	7.0	tetraacylated sulfoglycolipids(122:0)NH4+

2286.9118	7.0	tetraacylated sulfoglycolipids(124:0)Na+
2250.9021	7.0	tetraacylated sulfoglycolipids(123:0)H+
2240.8999	7.0	tetraacylated sulfoglycolipids(123:0)Na+ tetraacylated sulfoglycolipids(125:0)H+
2288.9124	7.0	tetraacylated sulfoglycolipids(126:0)H+
2253.8981	7.0	tetraacylated sulfoglycolipids(122:0)NH4+
2222.8766	7.0	tetraacylated sulfoglycolipids(123:0)Na+ tetraacylated sulfoglycolipids(121:0)H+
2223.8781	7.0	tetraacylated sulfoglycolipids(120:0)NH4+
2237.8895	7.0	tetraacylated sulfoglycolipids(121:0)NH4+
2225.8724	7.0	tetraacylated sulfoglycolipids(120:0)NH4+
2181.8275	7.1	tetraacylated sulfoglycolipids(117:0)NH4+
2156.7946	7.1	tetraacylated sulfoglycolipids(117:0)Na+
2170.8021	7.1	tetraacylated sulfoglycolipids(118:0)Na+
2168.8088	7.1	tetraacylated sulfoglycolipids(116:0)NH4+
2141.7775	7.1	tetraacylated sulfoglycolipids(114:0)NH4+
2166.8092	7.2	tetraacylated sulfoglycolipids(117:0)H+
2167.8006	7.2	tetraacylated sulfoglycolipids(116:0)NH4+
901.60383	7.0	mycobactins(21:1)NH4+
890.64487	7.0	lipopentapeptide(19:0)H+
912.61956	7.0	lipopentapeptide(19:0)Na+
876.61649	7.2	lipopentapeptide(18:0)H+
865.60929	7.3	lipopentapeptide(16:0)NH4+
898.61001	7.3	lipopentapeptide(18:0)Na+
935.68227	7.4	lipopentapeptide(21:0)NH4+
1378.0512	22.1	diacylated sulfoglycolipids(65:0)H+
1386.0191	22.1	diacylated sulfoglycolipids(64:0)Na+
1381.0593	22.1	diacylated sulfoglycolipids(64:0)NH4+
1364.0327	22.1	diacylated sulfoglycolipids(64:0)H+
1365.0359	22.1	diacylated sulfoglycolipids(63:0)NH4+
1379.0477	22.1	diacylated sulfoglycolipids(64:0)NH4+
1321.9814	22.2	diacylated sulfoglycolipids(61:0)H+
1357.9828	22.2	diacylated sulfoglycolipids(62:0)Na+
1343.9701	22.2	diacylated sulfoglycolipids(61:0)Na+
1339.0133	22.2	diacylated sulfoglycolipids(61:0)NH4+
1322.984	22.2	diacylated sulfoglycolipids(60:0)NH4+
1353.025	22.2	diacylated sulfoglycolipids(62:0)NH4+
1335.9997	22.2	diacylated sulfoglycolipids(62:0)H+
1337.0034	22.2	diacylated sulfoglycolipids(61:0)NH4+
1261.929	22.3	diacylated sulfoglycolipids(58:0)H+
1086.7339	22.3	diacylated sulfoglycolipids(43:0)NH4+
1301.9237	22.3	diacylated sulfoglycolipids(58:0)Na+
1294.9547	22.3	diacylated sulfoglycolipids(58:0)NH4+
1296.9675	22.3	diacylated sulfoglycolipids(58:0)NH4+
1315.9358	22.3	diacylated sulfoglycolipids(59:0)Na+
1310.9798	22.3	diacylated sulfoglycolipids(59:0)NH4+
1293.9559	22.3	diacylated sulfoglycolipids(59:0)H+
1280.9461	22.3	diacylated sulfoglycolipids(57:0)NH4+
1279.9421	22.3	diacylated sulfoglycolipids(58:0)H+
1259.881	22.5	diacylated sulfoglycolipids(55:0)Na+
1254.9197	22.5	diacylated sulfoglycolipids(55:0)NH4+
1252.9147	22.5	diacylated sulfoglycolipids(55:0)NH4+
1251.9082	22.5	diacylated sulfoglycolipids(56:0)H+
1273.8932	22.5	diacylated sulfoglycolipids(56:0)Na+
1268.9364	22.5	diacylated sulfoglycolipids(56:0)NH4+
1058.7034	22.5	diacylated sulfoglycolipids(41:0)NH4+
1238.8975	22.5	diacylated sulfoglycolipids(54:0)NH4+
1217.8263	22.6	diacylated sulfoglycolipids(52:0)Na+
1212.8715	22.6	diacylated sulfoglycolipids(52:0)NH4+
1175.7822	22.6	diacylated sulfoglycolipids(49:0)Na+
1170.8251	22.6	diacylated sulfoglycolipids(49:0)NH4+
1153.8032	22.6	diacylated sulfoglycolipids(49:0)H+
1142.7975	22.7	diacylated sulfoglycolipids(47:0)NH4+
1188.7965	22.7	diacylated sulfoglycolipids(50:0)Na+
1125.7701	22.7	diacylated sulfoglycolipids(47:0)H+
1147.7473	22.7	diacylated sulfoglycolipids(47:0)Na+

1184.8414	22.7	diacylated sulfoglycolipids(50:0)NH4+
911.65371	22.4	decaprenylphosphoribose(50:10)H+
933.63523	22.4	decaprenylphosphoribose(50:10)Na+ phosphatidylinositols(41:2)H+
761.58114	22.4	glucuronosyl diacylglycerol(32:0)H+ phosphatidylethanolamines(36:2)NH4+
806.6285	23.6	glucuronosyl diacylglycerol(34:0)NH4+
820.65772	25.9	glucuronosyl diacylglycerol(35:0)NH4+
817.64296	26.0	glucuronosyl diacylglycerol(36:0)H+ phosphatidylethanolamines(40:2)NH4+
907.66336	23.3	lipopentapeptide(19:0)NH4+
904.65996	23.3	lipopentapeptide(20:0)H+
919.74137	22.7	phosphatidylglycerols(46:0)H+
861.66454	22.9	phosphatidylglycerols(42:1)H+
810.61946	22.9	phosphatidylglycerols(37:0)NH4+
796.60554	23.0	phosphatidylglycerols(36:0)NH4+
808.60544	23.0	phosphatidylglycerols(37:1)NH4+
787.54435	23.1	phosphatidylglycerols(35:0)Na+
799.54667	23.1	phosphatidylglycerols(36:1)Na+
782.5897	23.1	phosphatidylglycerols(35:0)NH4+
777.5632	23.1	phosphatidylglycerols(36:1)H+
794.58949	23.1	phosphatidylglycerols(36:1)NH4+
765.56292	23.1	phosphatidylglycerols(35:0)H+
821.62484	23.1	phosphatidylglycerols(39:0)H+
785.53348	23.2	phosphatidylglycerols(35:1)Na+
807.61012	23.2	phosphatidylglycerols(38:0)H+
763.54759	23.2	phosphatidylglycerols(35:1)H+
773.52815	23.2	phosphatidylglycerols(34:0)Na+
780.5747	23.2	phosphatidylglycerols(35:1)NH4+
792.57456	23.2	phosphatidylglycerols(36:2)NH4+
751.54506	23.2	phosphatidylglycerols(34:0)H+
768.57054	23.2	phosphatidylglycerols(34:0)NH4+
850.64929	23.2	phosphatidylglycerols(40:1)NH4+
836.63411	23.2	phosphatidylglycerols(39:1)NH4+
822.61949	23.3	phosphatidylglycerols(38:1)NH4+
749.53233	23.3	phosphatidylglycerols(34:1)H+
766.55944	23.3	phosphatidylglycerols(34:1)NH4+
771.51433	23.3	phosphatidylglycerols(34:1)Na+
853.59113	23.3	phosphatidylglycerols(40:2)Na+
909.65566	23.3	phosphatidylglycerols(44:2)Na+
737.5327	23.3	phosphatidylglycerols(33:0)H+
754.55796	23.3	phosphatidylglycerols(33:0)NH4+
779.58091	23.3	phosphatidylglycerols(36:0)H+
869.61733	23.3	phosphatidylglycerols(41:1)Na+
805.60159	23.3	phosphatidylglycerols(38:1)H+
724.51924	23.3	phosphatidylglycerols(31:1)NH4+
752.54411	23.3	phosphatidylglycerols(33:1)NH4+
740.54246	23.3	phosphatidylglycerols(32:0)NH4+
735.51688	23.4	phosphatidylglycerols(33:1)H+
757.49943	23.4	phosphatidylglycerols(33:1)Na+
764.54349	23.4	phosphatidylglycerols(34:2)NH4+
747.51699	23.4	phosphatidylglycerols(34:2)H+
745.49829	23.4	phosphatidylglycerols(32:0)Na+
726.52747	23.4	phosphatidylglycerols(31:0)NH4+
820.61202	23.4	phosphatidylglycerols(38:2)NH4+
738.52781	23.4	phosphatidylglycerols(32:1)NH4+
721.50097	23.4	phosphatidylglycerols(32:1)H+
743.484	23.4	phosphatidylglycerols(32:1)Na+
717.46783	23.5	phosphatidylglycerols(30:0)Na+
712.51159	23.5	phosphatidylglycerols(30:0)NH4+
736.5159	23.5	phosphatidylglycerols(32:2)NH4+
615.34824	26.7	lyso phosphatidylinositols(19:0)H+
1561.1665	24.9	cardiolipins(78:3)NH4+
1467.0959	24.9	cardiolipins(71:1)NH4+
1470.0257	24.9	cardiolipins(71:2)Na+
1465.0851	24.9	cardiolipins(71:2)NH4+
1463.0674	24.9	cardiolipins(71:3)NH4+

1453.0784	24.9	cardiolipins(70:1)NH4+
1439.0701	24.9	cardiolipins(69:1)NH4+
1451.0683	24.9	cardiolipins(70:2)NH4+
1475.0851	24.9	cardiolipins(72:4)NH4+
1441.0766	25.0	cardiolipins(69:0)NH4+
1450.0598	25.0	cardiolipins(71:1)H+
1477.0803	25.0	cardiolipins(72:3)NH4+
1461.043	25.0	cardiolipins(71:4)NH4+
1448.0555	25.0	cardiolipins(70:3)NH4+ phosphatidylethanolamines dimer(34:2)NH4+
1438.0696	25.0	cardiolipins(70:0)H+
1432.025	25.0	cardiolipins(70:3)H+ phosphatidylethanolamines dimer(34:2)H+
1434.0375	25.0	cardiolipins(70:2)H+
1430.0052	25.0	cardiolipins(70:4)H+
1437.0558	25.0	cardiolipins(69:2)NH4+
1446.0443	25.0	cardiolipins(71:2)H+
1435.0403	25.0	cardiolipins(69:3)NH4+
1447.0376	25.0	cardiolipins(70:4)NH4+
1436.0446	25.0	cardiolipins(70:1)H+
1425.0477	25.0	cardiolipins(68:1)NH4+
1533.1341	25.0	cardiolipins(76:3)NH4+
1416.9914	25.0	cardiolipins(69:4)H+
1424.044	25.0	cardiolipins(69:0)H+
1523.1486	25.0	cardiolipins(75:1)NH4+
1423.0398	25.0	cardiolipins(68:2)NH4+
1519.1216	25.0	cardiolipins(75:3)NH4+
1531.1274	25.0	cardiolipins(76:4)NH4+
1521.1384	25.0	cardiolipins(75:2)NH4+
1406.0117	25.1	cardiolipins(68:2)H+
1407.0153	25.1	cardiolipins(67:3)NH4+
1505.1152	25.1	cardiolipins(74:3)NH4+ phosphatidylethanolamines dimer(36:2)NH4+
1413.0434	25.1	cardiolipins(67:0)NH4+
1408.0191	25.1	cardiolipins(68:1)H+
1503.1015	25.1	cardiolipins(74:4)NH4+
1411.0353	25.1	cardiolipins(67:1)NH4+
1399.0241	25.1	cardiolipins(66:0)NH4+
1421.0249	25.1	cardiolipins(68:3)NH4+
1422.0298	25.1	cardiolipins(69:1)H+
1409.0227	25.1	cardiolipins(67:2)NH4+
1403.9967	25.2	cardiolipins(66:0)Na+ cardiolipins(68:3)H+
1405.0012	25.2	cardiolipins(67:4)NH4+
1385.0102	25.2	cardiolipins(65:0)NH4+
1397.017	25.2	cardiolipins(66:1)NH4+
1395.0075	25.2	cardiolipins(66:2)NH4+
1378.9829	25.2	cardiolipins(65:3)NH4+
1377.9792	25.2	cardiolipins(66:2)H+
1419.0086	25.2	cardiolipins(68:4)NH4+
1379.9886	25.2	cardiolipins(66:1)H+
1354.9774	25.2	cardiolipins(63:1)NH4+
1383.003	25.3	cardiolipins(65:1)NH4+
1380.9911	25.3	cardiolipins(65:2)NH4+
1393.9973	25.3	cardiolipins(67:1)H+
1392.993	25.3	cardiolipins(66:3)NH4+ phosphatidylethanolamines dimer(32:2)NH4+
1401.9804	25.3	cardiolipins(66:1)Na+ cardiolipins(68:4)H+
1375.9643	25.3	cardiolipins(66:3)H+ phosphatidylethanolamines dimer(32:2)H+
1376.9684	25.3	cardiolipins(65:4)NH4+
1433.0178	25.3	cardiolipins(69:4)NH4+
1368.9863	25.3	cardiolipins(64:1)NH4+
1361.9395	25.3	cardiolipins(63:0)Na+ cardiolipins(65:3)H+
1348.9468	25.3	cardiolipins(64:2)H+
1350.9486	25.3	cardiolipins(63:3)NH4+
1366.9745	25.3	cardiolipins(64:2)NH4+
1390.9765	25.3	cardiolipins(66:4)NH4+
1348.935	25.3	cardiolipins(63:4)NH4+
1364.96	25.3	cardiolipins(64:3)NH4+

1373.9479	25.3	cardiolipins(66:4)H+
1347.9307	25.3	cardiolipins(64:3)H+
1278.853	25.4	cardiolipins(58:4)NH4+
1371.9409	25.4	cardiolipins(64:2)Na+
1362.9429	25.4	cardiolipins(64:4)NH4+
1511.1768	25.6	cardiolipins(74:0)NH4+
1494.1434	25.6	cardiolipins(74:0)H+
1502.1135	25.7	cardiolipins(73:0)Na+ cardiolipins(75:3)H+
1483.1119	25.7	cardiolipins(73:2)NH4+
1480.1308	25.7	cardiolipins(73:0)H+
1491.1146	25.7	cardiolipins(73:3)NH4+
1490.1107	25.7	cardiolipins(74:2)H+ phosphatidylethanolamines dimer(35:0)Na+
1488.0983	25.7	cardiolipins(73:4)NH4+
1476.096	25.8	cardiolipins(73:2)H+
1478.0903	25.8	cardiolipins(73:1)H+
1258.8856	25.9	cardiolipins(56:0)NH4+
1180.7502	26.2	cardiolipins(51:4)NH4+
1270.8827	24.7	monoacyl phosphatidylinositol monomannosides(51:0)NH4+
1537.1372	24.9	diacyl phosphatidylinositol monomannosides(69:0)NH4+
1534.138	25.0	diacyl phosphatidylinositol monomannosides(70:0)H+
1509.1278	25.0	diacyl phosphatidylinositol monomannosides(67:0)NH4+
1520.1267	25.0	diacyl phosphatidylinositol monomannosides(69:0)H+
1698.2024	25.5	diacyl phosphatidylinositol dimannosides(69:0)NH4+
1713.2207	25.5	diacyl phosphatidylinositol dimannosides(70:0)NH4+
1432.9447	27.4	monoacyl phosphatidylinositol dimannosides(51:0)NH4+
1460.9745	27.5	monoacyl phosphatidylinositol dimannosides(53:0)NH4+
832.67399	25.5	phosphatidic acids(44:1)NH4+ phosphatidylethanolamines(42:0)H+
776.61546	25.5	phosphatidic acids(40:1)NH4+ phosphatidylethanolamines(38:0)H+
762.59949	25.6	phosphatidic acids(39:1)NH4+ phosphatidylethanolamines(37:0)H+
760.58383	25.6	phosphatidic acids(39:2)NH4+ phosphatidylethanolamines(37:1)H+
748.58493	25.6	phosphatidic acids(38:1)NH4+ phosphatidylethanolamines(36:0)H+
746.5687	25.7	phosphatidic acids(38:2)NH4+ phosphatidylethanolamines(36:1)H+
734.57145	25.7	phosphatidic acids(37:1)NH4+ phosphatidylethanolamines(35:0)H+
720.55555	25.8	phosphatidic acids(36:1)NH4+ phosphatidic acids(36:1)NH4+ phosphatidylethanolamines(34:0)H+
732.55333	25.8	phosphatidic acids(37:2)NH4+ phosphatidylethanolamines(35:1)H+
742.53452	25.8	phosphatidic acids(38:4)NH4+ phosphatidylethanolamines(34:0)Na+
764.52112	25.9	phosphatidic acids(40:7)NH4+
718.53837	25.9	phosphatidic acids(36:2)NH4+ phosphatidylethanolamines(34:1)H+
706.5381	26.0	phosphatidic acids(35:1)NH4+ phosphatidylethanolamines(33:0)H+
740.51974	26.0	phosphatidic acids(38:5)NH4+ phosphatidylethanolamines(34:1)Na+
692.52366	26.1	phosphatidic acids(34:1)NH4+ phosphatidylethanolamines(32:0)H+
704.52182	26.1	phosphatidic acids(35:2)NH4+ phosphatidylethanolamines(33:1)H+
809.60098	26.1	phosphatidic acids(42:1)Na+
714.50374	26.1	phosphatidic acids(36:4)NH4+ phosphatidylethanolamines(32:0)Na+
716.52112	26.1	phosphatidic acids(36:3)NH4+ phosphatidylethanolamines(34:2)H+
690.5065	26.2	phosphatidic acids(34:2)NH4+ phosphatidylethanolamines(32:1)H+
678.50607	26.2	phosphatidic acids(33:1)NH4+ phosphatidylethanolamines(31:0)H+
676.49175	26.3	phosphatidic acids(33:2)NH4+ phosphatidylethanolamines(31:1)H+
664.49074	26.3	phosphatidic acids(32:1)NH4+ phosphatidylethanolamines(30:0)H+
650.47414	26.4	phosphatidic acids(31:1)NH4+ phosphatidylethanolamines(29:0)H+
662.47496	26.4	phosphatidic acids(32:2)NH4+ phosphatidylethanolamines(30:1)H+
777.61836	25.5	phosphatidylethanolamines(37:1)NH4+
782.56982	25.5	phosphatidylethanolamines(37:1)Na+
765.6062	25.6	phosphatidylethanolamines(36:0)NH4+
763.60337	25.6	phosphatidylethanolamines(36:1)NH4+
908.70422	25.6	phosphatidylethanolamines(46:1)Na+
770.5665	25.6	phosphatidylethanolamines(36:0)Na+
761.5873	25.6	phosphatidylethanolamines(36:2)NH4+
751.58346	25.6	phosphatidylethanolamines(35:0)NH4+
866.66417	25.6	phosphatidylethanolamines(43:1)Na+
1496.1596	25.6	phosphatidylethanolamines dimer(36:0)H+
1485.1545	25.7	phosphatidylethanolamines dimer(35:0)NH4+
894.68082	25.7	phosphatidylethanolamines(45:1)Na+
852.64952	25.7	phosphatidylethanolamines(42:1)Na+

768.55232	25.7	phosphatidylethanolamines(36:1)Na+
756.55051	25.7	phosphatidylethanolamines(35:0)Na+
747.57181	25.7	phosphatidylethanolamines(35:2)NH4+
1481.1344	25.7	phosphatidylethanolamines dimer(35:1)NH4+ phosphatidylethanolamines dimer(35:1)NH4+
1468.133	25.7	phosphatidylethanolamines dimer(35:0)H+
737.57768	25.7	phosphatidylethanolamines(34:0)NH4+
880.674	25.8	phosphatidylethanolamines(44:1)Na+
1457.1251	25.8	phosphatidylethanolamines dimer(34:0)NH4+
1477.0973	25.8	phosphatidylethanolamines dimer(35:2)NH4+
1466.0896	25.8	phosphatidylethanolamines dimer(36:2)H+
833.67029	25.8	phosphatidylethanolamines(41:1)NH4+
838.63461	25.8	phosphatidylethanolamines(41:1)Na+
754.53405	25.8	phosphatidylethanolamines(35:1)Na+
723.56194	25.8	phosphatidylethanolamines(33:0)NH4+
1440.1007	25.8	phosphatidylethanolamines dimer(34:0)H+
1453.1038	25.9	phosphatidylethanolamines dimer(34:1)NH4+
1464.0936	25.9	phosphatidylethanolamines dimer(35:1)H+ phosphatidylethanolamines dimer(35:1)H+
1462.0806	25.9	phosphatidylethanolamines dimer(34:0)Na+
1460.0867	25.9	phosphatidylethanolamines dimer(35:2)H+
819.65615	25.9	phosphatidylethanolamines(40:1)NH4+
836.62161	25.9	phosphatidylethanolamines(41:2)Na+
709.54638	26.0	phosphatidylethanolamines(32:0)NH4+
728.51992	26.0	phosphatidylethanolamines(33:0)Na+
1436.0858	26.0	phosphatidylethanolamines dimer(34:1)H+
1401.0802	26.0	phosphatidylethanolamines dimer(32:0)NH4+
1384.0401	26.1	phosphatidylethanolamines dimer(32:0)H+
695.53109	26.1	phosphatidylethanolamines(31:0)NH4+
1397.0381	26.1	phosphatidylethanolamines dimer(34:1)NH4+
791.62669	26.1	phosphatidylethanolamines(38:1)NH4+
1458.0825	26.2	phosphatidylethanolamines dimer(34:1)Na+
700.48636	26.2	phosphatidylethanolamines(31:0)Na+
712.48792	26.2	phosphatidylethanolamines(32:1)Na+
667.60063	26.3	phosphatidylethanolamines(29:0)NH4+
686.47163	26.3	phosphatidylethanolamines(30:0)Na+
688.49007	26.4	phosphatidylethanolamines(32:2)H+
663.4721	26.4	phosphatidylethanolamines(29:2)NH4+
749.57509	26.6	phosphatidylethanolamines(35:1)NH4+
994.72969	26.2	phosphatidylinositols(44:1)NH4+
903.58969	26.4	phosphatidylinositols(37:0)Na+
881.6094	26.4	phosphatidylinositols(37:0)H+
898.63658	26.4	phosphatidylinositols(37:0)NH4+
889.57549	26.5	phosphatidylinositols(36:0)Na+
910.63705	26.5	phosphatidylinositols(38:1)NH4+
867.5953	26.5	phosphatidylinositols(36:0)H+
884.6205	26.5	phosphatidylinositols(36:0)NH4+
879.59314	26.5	phosphatidylinositols(37:1)H+
896.62179	26.5	phosphatidylinositols(37:1)NH4+
908.62065	26.6	phosphatidylinositols(38:2)NH4+
875.56218	26.6	phosphatidylinositols(35:0)Na+
882.60776	26.6	phosphatidylinositols(36:1)NH4+
880.5917	26.6	phosphatidylinositols(36:2)NH4+
853.58113	26.6	phosphatidylinositols(35:0)H+
870.60848	26.6	phosphatidylinositols(35:0)NH4+
865.58037	26.6	phosphatidylinositols(36:1)H+
952.66377	26.7	phosphatidylinositols(41:1)NH4+
971.65971	26.7	phosphatidylinositols(42:1)Na+
854.58359	26.7	phosphatidylinositols(34:1)NH4+
938.66124	26.8	phosphatidylinositols(40:1)NH4+
861.54507	26.8	phosphatidylinositols(34:0)Na+
856.59028	26.8	phosphatidylinositols(34:0)NH4+
868.59167	26.8	phosphatidylinositols(35:1)NH4+
851.56449	26.8	phosphatidylinositols(35:1)H+
839.56381	26.8	phosphatidylinositols(34:0)H+
840.5666	26.9	phosphatidylinositols(33:1)NH4+

837.54894	26.9	phosphatidylinositols(34:1)H+
825.54843	26.9	phosphatidylinositols(33:0)H+
847.53017	27.0	phosphatidylinositols(33:0)Na+
842.57513	27.0	phosphatidylinositols(33:0)NH4+
1013.7013	27.0	phosphatidylinositols(45:1)Na+
1011.6854	27.0	phosphatidylinositols(45:2)Na+
866.57716	27.0	phosphatidylinositols(35:2)NH4+
826.55011	27.1	phosphatidylinositols(32:1)NH4+
828.5594	27.1	phosphatidylinositols(32:0)NH4+
811.53327	27.1	phosphatidylinositols(32:0)H+
852.56407	27.1	phosphatidylinositols(34:2)NH4+
835.53366	27.2	phosphatidylinositols(34:2)H+
814.54383	27.2	phosphatidylinositols(31:0)NH4+
797.52056	27.2	phosphatidylinositols(31:0)H+
809.51796	27.2	phosphatidylinositols(32:1)H+
783.50162	27.3	phosphatidylinositols(30:0)H+
800.52885	27.4	phosphatidylinositols(30:0)NH4+
824.53087	27.4	phosphatidylinositols(32:2)NH4+
369.20546	30.4	lyso phosphatidic acids(13:0)H+
383.22075	30.3	lyso phosphatidic acids(14:0)H+
397.23704	30.4	lyso phosphatidic acids(15:0)H+
411.25178	30.3	lyso phosphatidic acids(16:0)H+
454.29278	30.6	lyso phosphatidic acids(18:1)NH4+ lyso phosphatidylethanolamines(16:0)H+
482.32413	30.9	lyso phosphatidic acids(20:1)NH4+ lyso phosphatidylethanolamines(18:0)H+
496.33968	30.8	lyso phosphatidic acids(21:1)NH4+ lyso phosphatidylethanolamines(19:0)H+
510.35483	30.7	lyso phosphatidic acids(22:1)NH4+ lyso phosphatidylethanolamines(20:0)H+
426.26046	31.9	lyso phosphatidylethanolamines(14:0)H+
454.29281	31.3	lyso phosphatidylethanolamines(16:0)H+
476.27527	31.3	lyso phosphatidylethanolamines(16:0)Na+
452.27713	31.6	lyso phosphatidylethanolamines(16:1)H+
468.30823	31.1	lyso phosphatidylethanolamines(17:0)H+
504.30612	31.0	lyso phosphatidylethanolamines(18:0)Na+
480.30849	31.2	lyso phosphatidylethanolamines(18:1)H+
518.32161	30.8	lyso phosphatidylethanolamines(19:0)Na+
494.32619	31.2	lyso phosphatidylethanolamines(19:1)H+
330.15919	32.8	monoglycosyl parahydroxybenzoic acid derivatives(0:0)NH4+
272.25835	32.6	unsaturated fatty acids(16:1)NH4+
300.28919	32.1	unsaturated fatty acids(18:1)NH4+

Negative-ion mode *M. tuberculosis H37Rv* dataset: 366 annotated features, 5240 features remain unannotated, 5606 features total

Median *m/z*	Median RT(minutes)	Annotation(10ppm)
1108.1323	3.6	alpha mycolic acids(76:0, 1 or 2)H-
1136.1636	3.6	alpha mycolic acids(78:0, 1 or 2)H-
1196.2190	3.6	methoxy mycolic acids(81:0 or 1)H-
1224.2519	3.6	methoxy mycolic acids(83:0 or 1)H-
1252.2830	3.6	methoxy mycolic acids(85:0 or 1)H-
1280.3133	3.6	methoxy mycolic acids(87:0 or 1)H-
1164.1945	3.6	alpha mycolic acids(80:0, 1 or 2)H-
1412.3865	3.6	phthiocerol dimycocerosates(PDIMA and A')(59:0)HCOO- phthiocerol dimycocerosates(PDIMA and A')(58:0)CH3COO- phthiocerol dimycocerosates(PDIMA and A')(57:0)HCOO- phthiocerol dimycocerosates(PDIMA and A')(56:0)CH3COO- phthiocerol dimycocerosates(PDIMA and A')(57:0)CH3COO- phthiocerol dimycocerosates(PDIMA and A')(58:0)HCOO- phthiocerol dimycocerosates(PDIMA and A')(56:0)HCOO- phthiotriol dimycocerosates(59:0)CH3COO- phthiotriol dimycocerosates(57:0)HCOO-
1440.4189	3.6	phthiocerol dimycocerosates(PDIMA and A')(60:0)CH3COO- phthiocerol dimycocerosates(PDIMA and A')(61:0)HCOO- phthiocerol dimycocerosates(PDIMA and A')(59:0)HCOO- phthiocerol dimycocerosates(PDIMA and A')(58:0)CH3COO- phthiocerol dimycocerosates(PDIMA and A')(60:0)HCOO- phthiocerol dimycocerosates(PDIMA and A')(59:0)CH3COO- phthiocerol dimycocerosates(PDIMA and A')(57:0)CH3COO- phthiocerol dimycocerosates(PDIMA and A')(58:0)HCOO- phthiotriol dimycocerosates(61:0)CH3COO- phthiotriol dimycocerosates(59:0)HCOO-

		phthiocerol dimycocerosates(PDIMA and A')(60:0)HCOO- phthiocerol dimycocerosates(PDIMA and A')(59:0)CH3COO-
		phthiocerol dimycocerosates(PDIMA and A')(57:0)CH3COO- phthiocerol dimycocerosates(PDIMA and A')(58:0)HCOO-
1426.4001	3.6	phthiocerol dimycocerosates(PDIMA and A')(59:0)HCOO- phthiocerol dimycocerosates(PDIMA and A')(58:0)CH3COO-
		phthiocerol dimycocerosates(PDIMA and A')(57:0)HCOO- phthiocerol dimycocerosates(PDIMA and A')(56:0)CH3COO-
		phthiotriol dimycocerosates(57:0)CH3COO- phthiotriol dimycocerosates(61:0)HCOO-
		phthiocerol dimycocerosates(PDIMA and A')(62:0)HCOO- phthiocerol dimycocerosates(PDIMA and A')(61:0)CH3COO-
		phthiocerol dimycocerosates(PDIMA and A')(60:0)HCOO- phthiocerol dimycocerosates(PDIMA and A')(59:0)CH3COO-
1454.4323	3.5	phthiocerol dimycocerosates(PDIMA and A')(60:0)CH3COO- phthiocerol dimycocerosates(PDIMA and A')(61:0)HCOO-
		phthiocerol dimycocerosates(PDIMA and A')(59:0)HCOO- phthiocerol dimycocerosates(PDIMA and A')(58:0)CH3COO-
		phthiotriol dimycocerosates(59:0)CH3COO- phthiotriol dimycocerosates(63:0)HCOO-
1306.1624	4.3	glucose monomycolate methoxy(74:0 or 1)HCOO- glucose monomycolate methoxy(73:1)CH3COO-
1316.1908	4.2	glucose monomycolatealpha(75:1 or 2)CH3COO- glucose monomycolatealpha(76:0, 1 or 2)HCOO-
1334.1943	4.3	glucose monomycolate methoxy(75:0 or 1)CH3COO- glucose monomycolate methoxy(76:0 or 1)HCOO-
1344.2215	3.9	glucose monomycolatealpha(77:1 or 2)CH3COO- glucose monomycolatealpha(78:0, 1 or 2)HCOO-
1460.3396	3.9	glucose monomycolate methoxy(84:0 or 1)CH3COO- glucose monomycolate methoxy(85:0 or 1)HCOO-
585.4718	4.0	diacylglycerols(30:0)HCOO- diacylglycerols(30:0)HCOO-
611.4893	3.9	diacylglycerols(32:1)HCOO-
613.5048	3.9	diacylglycerols(32:0)HCOO-
625.5035	3.9	diacylglycerols(32:1)CH3COO-
627.5165	3.8	diacylglycerols(32:0)CH3COO- diacylglycerols(33:0)HCOO-
637.5050	3.9	diacylglycerols(34:2)HCOO-
639.5208	3.9	diacylglycerols(34:1)HCOO-
641.5350	3.9	diacylglycerols(33:0)CH3COO- diacylglycerols(34:0)HCOO-
653.5356	3.9	diacylglycerols(34:1)CH3COO- diacylglycerols(35:1)HCOO-
655.5514	3.9	diacylglycerols(34:0)CH3COO- diacylglycerols(35:0)HCOO-
665.5356	4.0	diacylglycerols(36:2)HCOO-
667.5515	3.9	diacylglycerols(35:1)CH3COO- diacylglycerols(36:1)HCOO-
669.5666	3.9	diacylglycerols(35:0)CH3COO- diacylglycerols(36:0)HCOO-
681.5657	3.9	diacylglycerols(36:1)CH3COO- diacylglycerols(37:1)HCOO-
697.5983	3.9	diacylglycerols(37:0)CH3COO- diacylglycerols(38:0)HCOO-
725.6305	3.9	diacylglycerols(39:0)CH3COO- diacylglycerols(40:0)HCOO- diacylglycerols(40:0)HCOO-
375.2753	4.8	monoacylglycerols(16:0)HCOO-
401.2914	4.8	monoacylglycerols(18:1)HCOO-
403.3058	4.7	monoacylglycerols(18:0)HCOO-
417.3213	4.8	monoacylglycerols(18:0)CH3COO- monoacylglycerols(19:0)HCOO-
1386.2855	3.6	monomeromycolyl diacylglycerols(84:0)CH3COO- monomeromycolyl diacylglycerols(84:0)CH3COO-
1320.2790	3.8	monomeromycolyl diacylglycerols(86:0)H-
1394.3023	3.7	monomeromycolyl diacylglycerols(86:0)CH3COO- monomeromycolyl diacylglycerols(87:0)HCOO-
1392.3101	3.7	monomeromycolyl diacylglycerols(86:1)CH3COO- monomeromycolyl diacylglycerols(87:1)HCOO-
1388.3410	3.5	monomeromycolyl diacylglycerols(90:1)H-
1400.3408	3.7	monomeromycolyl diacylglycerols(91:2)H-
1432.3937	3.6	monomeromycolyl diacylglycerols(93:0)H-
1414.3863	3.5	glycerol monomycolate methoxy(87:0 or 1)CH3COO- glycerol monomycolate methoxy(88:0 or 1)HCOO-
1428.3945	3.6	glycerol monomycolate methoxy(88:0 or 1)CH3COO- glycerol monomycolate methoxy(89:0 or 1)HCOO-
467.4453	4.3	hydroxyphthioceranic acids(30:0)H-
906.5916	6.1	lipopentapeptide(16:0)CH3COO- lipopentapeptide(17:0)HCOO-
920.6200	5.9	lipopentapeptide(17:0)CH3COO- lipopentapeptide(18:0)HCOO-
860.5867	6.0	lipopentapeptide(17:0)H-
877.5884	6.3	diacyltrehaloses(33:1)HCOO- diacyltrehaloses(32:0)CH3COO-
887.5787	5.8	diacyltrehaloses(34:2)HCOO- diacyltrehaloses(33:1)CH3COO-
889.5929	6.1	diacyltrehaloses(34:2)HCOO- diacyltrehaloses(33:1)CH3COO-
917.6236	5.9	diacyltrehaloses(36:2)HCOO- diacyltrehaloses(35:1)CH3COO- diacyltrehaloses(36:0)HCOO-
939.6097	6.0	diacyltrehaloses(38:4)HCOO-
943.6407	6.0	diacyltrehaloses(38:2)HCOO- diacyltrehaloses(37:1)CH3COO-
953.6193	5.9	diacyltrehaloses(38:4)CH3COO-
955.6431	5.9	diacyltrehaloses(38:3)CH3COO- decaprenylphosphoribose(50:10)HCOO-
1003.7270	6.4	diacyltrehaloses(42:0)HCOO-
1017.7394	6.5	diacyltrehaloses(42:0)CH3COO- diacyltrehaloses(43:0)HCOO-
1520.2622	6.7	triacyltrehaloses(77:1)CH3COO- triacyltrehaloses(78:1)HCOO-
1562.3129	6.6	triacyltrehaloses(80:1)CH3COO- triacyltrehaloses(81:1)HCOO-
1650.4206	6.3	trehalose monomycolate methoxy(86:0 or 1)CH3COO- trehalose monomycolate methoxy(87:0 or 1)HCOO-
1590.3618	6.3	trehalose monomycolate alpha(83:1 or 2)CH3COO- trehalose monomycolate alpha(84:0, 1 or 2)HCOO-
1622.3921	6.4	trehalose monomycolate methoxy(84:0 or 1)CH3COO- trehalose monomycolate methoxy(85:0 or 1)HCOO-
1564.3338	6.5	trehalose monomycolateketo(80:0 or 1)CH3COO- trehalose monomycolateketo(81:0 or 1)HCOO-

1552.3049	6.5	trehalose monomycolate methoxy(79:0 or 1)CH3COO- trehalose monomycolate methoxy(80:0 or 1)HCOO-
1594.3618	6.5	trehalose monomycolate methoxy(82:0 or 1)CH3COO- trehalose monomycolate methoxy(83:0 or 1)HCOO-
1524.2758	6.6	trehalose monomycolate methoxy(77:0 or 1)CH3COO- trehalose monomycolate methoxy(78:0 or 1)HCOO-
1496.2461	6.6	trehalose monomycolate methoxy(75:0 or 1)CH3COO- trehalose monomycolate methoxy(76:0 or 1)HCOO-
1536.3017	6.6	trehalose monomycolateketo(78:0 or 1)CH3COO- trehalose monomycolateketo(79:0 or 1)HCOO-
1534.2943	6.6	trehalose monomycolate alpha(79:1 or 2)CH3COO- trehalose monomycolate alpha(80:0, 1 or 2)HCOO-
1538.2948	6.6	trehalose monomycolate methoxy(78:0 or 1)CH3COO- trehalose monomycolate methoxy(79:0 or 1)HCOO-
1566.3279	6.6	trehalose monomycolate methoxy(80:0 or 1)CH3COO- trehalose monomycolate methoxy(81:0 or 1)HCOO-
1506.2720	6.7	trehalose monomycolate alpha(77:1 or 2)CH3COO- trehalose monomycolate alpha(78:0, 1 or 2)HCOO-
1510.2740	6.7	trehalose monomycolate methoxy(76:0 or 1)CH3COO- trehalose monomycolate methoxy(77:0 or 1)HCOO-
1482.2413	6.7	trehalose monomycolate methoxy(74:0 or 1)CH3COO- trehalose monomycolate methoxy(75:0 or 1)HCOO-
1468.2179	6.7	trehalose monomycolate methoxy(74:0 or 1)HCOO- trehalose monomycolate methoxy(73:1)CH3COO-
1478.2421	6.7	trehalose monomycolate alpha(75:1 or 2)CH3COO- trehalose monomycolate alpha(76:0, 1 or 2)HCOO-
1450.2122	6.7	trehalose monomycolate alpha(73:0, 1 or 2)CH3COO- trehalose monomycolate alpha(74:0, 1 or 2)HCOO-
1454.2066	6.8	trehalose monomycolate methoxy(73:1)HCOO-
855.5769	26.5	diglycosylated diacylglycerol(30:0)H-
901.5828	4.8	diglycosylated diacylglycerol(30:0)HCOO-
2627.3193	6.8	tetraacylated sulfoglycolipids(150:0)H-
2641.3399	6.8	tetraacylated sulfoglycolipids(151:0)H-
2585.2719	6.8	tetraacylated sulfoglycolipids(147:0)H-
2613.3045	6.8	tetraacylated sulfoglycolipids(149:0)H-
2599.2862	6.8	tetraacylated sulfoglycolipids(148:0)H-
2555.2319	6.8	tetraacylated sulfoglycolipids(145:0)H-
2569.2360	6.9	tetraacylated sulfoglycolipids(146:0)H-
2443.1246	6.9	tetraacylated sulfoglycolipids(138:0)H-
2571.2584	6.9	tetraacylated sulfoglycolipids(146:0)H-
2583.2639	6.9	tetraacylated sulfoglycolipids(148:0)H- tetraacylated sulfoglycolipids(147:0)H-
2513.1945	6.9	tetraacylated sulfoglycolipids(143:0)H-
2533.2159	6.9	tetraacylated sulfoglycolipids(146:0)H-
2557.2409	6.9	tetraacylated sulfoglycolipids(145:0)H-
2529.2132	6.9	tetraacylated sulfoglycolipids(143:0)H-
2543.2267	6.9	tetraacylated sulfoglycolipids(144:0)H-
2541.2183	6.9	tetraacylated sulfoglycolipids(145:0)H- tetraacylated sulfoglycolipids(144:0)H-
2485.1598	6.9	tetraacylated sulfoglycolipids(141:0)H- tetraacylated sulfoglycolipids(140:0)H-
1996.6204	7.7	tetraacylated sulfoglycolipids(105:0)H-
2024.6569	7.5	tetraacylated sulfoglycolipids(107:0)H-
2038.6663	7.5	tetraacylated sulfoglycolipids(108:0)H-
2052.6830	7.5	tetraacylated sulfoglycolipids(109:0)H-
2050.6883	8.0	tetraacylated sulfoglycolipids(110:0)H-
2066.7069	7.4	tetraacylated sulfoglycolipids(110:0)H-
2080.7154	7.4	tetraacylated sulfoglycolipids(111:0)H-
2094.7296	7.4	tetraacylated sulfoglycolipids(112:0)H-
2078.7318	7.2	tetraacylated sulfoglycolipids(112:0)H-
2108.7535	7.3	tetraacylated sulfoglycolipids(113:0)H-
2136.7759	7.4	tetraacylated sulfoglycolipids(115:0)H-
2120.7769	7.2	tetraacylated sulfoglycolipids(115:0)H-
2150.7982	7.3	tetraacylated sulfoglycolipids(116:0)H-
2148.8033	7.2	tetraacylated sulfoglycolipids(117:0)H-
2164.8094	7.3	tetraacylated sulfoglycolipids(117:0)H-
2006.6338	8.0	tetraacylated sulfoglycolipids(107:0)H-
2006.6452	8.0	tetraacylated sulfoglycolipids(107:0)H-
2036.6684	7.9	tetraacylated sulfoglycolipids(109:0)H-
2048.6818	8.0	tetraacylated sulfoglycolipids(110:0)H-
2092.7472	7.2	tetraacylated sulfoglycolipids(113:0)H-
2106.7652	7.2	tetraacylated sulfoglycolipids(114:0)H-
2122.7691	7.3	tetraacylated sulfoglycolipids(114:0)H-
2104.7446	7.8	tetraacylated sulfoglycolipids(114:0)H-
2134.7864	7.4	tetraacylated sulfoglycolipids(116:0)H-
2132.7757	7.7	tetraacylated sulfoglycolipids(116:0)H-
2162.7970	7.3	tetraacylated sulfoglycolipids(117:0)H-
2146.7801	7.5	tetraacylated sulfoglycolipids(117:0)H-
2178.8281	7.2	tetraacylated sulfoglycolipids(118:0)H-
2176.8199	7.2	tetraacylated sulfoglycolipids(119:0)H- tetraacylated sulfoglycolipids(118:0)H-
2190.8504	7.1	tetraacylated sulfoglycolipids(120:0)H-

2206.8617	7.2	tetraacylated sulfoglycolipids(120:0)H-
2202.8350	7.3	tetraacylated sulfoglycolipids(121:0)H-
2220.8694	7.2	tetraacylated sulfoglycolipids(121:0)H-
2204.8638	7.1	tetraacylated sulfoglycolipids(121:0)H-
2218.8752	7.1	tetraacylated sulfoglycolipids(122:0)H-
2232.8895	7.1	tetraacylated sulfoglycolipids(123:0)H-
2248.8976	7.2	tetraacylated sulfoglycolipids(123:0)H-
2230.8968	7.0	tetraacylated sulfoglycolipids(123:0)H-
2244.8864	7.0	tetraacylated sulfoglycolipids(124:0)H-
2262.9130	7.2	tetraacylated sulfoglycolipids(124:0)H-
2246.9128	7.0	tetraacylated sulfoglycolipids(124:0)H-
2258.8222	7.0	tetraacylated sulfoglycolipids(125:0)H-
2260.8233	7.0	tetraacylated sulfoglycolipids(125:0)H-
2276.9407	7.1	tetraacylated sulfoglycolipids(125:0)H-
2274.9128	7.2	tetraacylated sulfoglycolipids(125:0)H-
2238.8670	7.1	tetraacylated sulfoglycolipids(125:0)H-
2290.9472	7.1	tetraacylated sulfoglycolipids(126:0)H-
2274.9493	7.0	tetraacylated sulfoglycolipids(126:0)H-
2272.9205	7.1	tetraacylated sulfoglycolipids(126:0)H-
2286.9434	7.0	tetraacylated sulfoglycolipids(127:0)H-
2304.9659	7.1	tetraacylated sulfoglycolipids(127:0)H-
2288.9628	7.0	tetraacylated sulfoglycolipids(127:0)H-
2316.9775	7.0	tetraacylated sulfoglycolipids(128:0)H-
2318.9935	7.0	tetraacylated sulfoglycolipids(128:0)H-
2302.9660	7.0	tetraacylated sulfoglycolipids(128:0)H-
2280.9321	7.1	tetraacylated sulfoglycolipids(128:0)H-
2332.9979	7.0	tetraacylated sulfoglycolipids(129:0)H-
2314.9745	7.0	tetraacylated sulfoglycolipids(129:0)H-
2328.9452	7.1	tetraacylated sulfoglycolipids(129:0)H-
2347.0192	7.0	tetraacylated sulfoglycolipids(130:0)H-
2331.0016	7.0	tetraacylated sulfoglycolipids(130:0)H-
2361.0265	7.0	tetraacylated sulfoglycolipids(131:0)H-
2345.0192	6.9	tetraacylated sulfoglycolipids(131:0)H-
2343.0029	7.0	tetraacylated sulfoglycolipids(131:0)H-
2322.9837	7.0	tetraacylated sulfoglycolipids(131:0)H-
2357.0241	6.9	tetraacylated sulfoglycolipids(132:0)H-
2359.0374	6.9	tetraacylated sulfoglycolipids(132:0)H-
2388.0601	7.0	tetraacylated sulfoglycolipids(133:0)H-
2373.0523	6.9	tetraacylated sulfoglycolipids(133:0)H-
2403.0855	7.0	tetraacylated sulfoglycolipids(134:0)H
2387.0638	6.9	tetraacylated sulfoglycolipids(134:0)H-
2365.0282	7.0	tetraacylated sulfoglycolipids(134:0)H-
2417.0979	7.0	tetraacylated sulfoglycolipids(135:0)H-
2401.0711	6.9	tetraacylated sulfoglycolipids(135:0)H-
2429.0916	7.0	tetraacylated sulfoglycolipids(136:0)H-
2431.0990	7.0	tetraacylated sulfoglycolipids(136:0)H-
2415.0845	7.0	tetraacylated sulfoglycolipids(136:0)H- tetraacylated sulfoglycolipids(135:0)H-
2445.1245	6.9	tetraacylated sulfoglycolipids(137:0)H-
2407.0835	7.0	tetraacylated sulfoglycolipids(137:0)H-
2457.1172	7.0	tetraacylated sulfoglycolipids(138:0)H-
2459.1380	6.9	tetraacylated sulfoglycolipids(138:0)H-
2455.0919	7.0	tetraacylated sulfoglycolipids(138:0)H-
2473.1542	6.9	tetraacylated sulfoglycolipids(139:0)H-
2471.1367	7.0	tetraacylated sulfoglycolipids(139:0)H-
2487.1697	6.9	tetraacylated sulfoglycolipids(140:0)H-
2449.1272	6.9	tetraacylated sulfoglycolipids(140:0)H-
2501.1847	6.9	tetraacylated sulfoglycolipids(141:0)H-
2499.1619	7.0	tetraacylated sulfoglycolipids(141:0)H-
2515.2001	6.9	tetraacylated sulfoglycolipids(142:0)H-
2527.1897	6.9	tetraacylated sulfoglycolipids(143:0)H-
2491.1737	6.9	tetraacylated sulfoglycolipids(143:0)H-
881.5746	11.1	sulfomenaquinones(45:8)H-
881.5741	7.1	sulfomenaquinones(45:8)H-
684.3197	8.1	dideoxycarboxymycobactins(7:1)H-

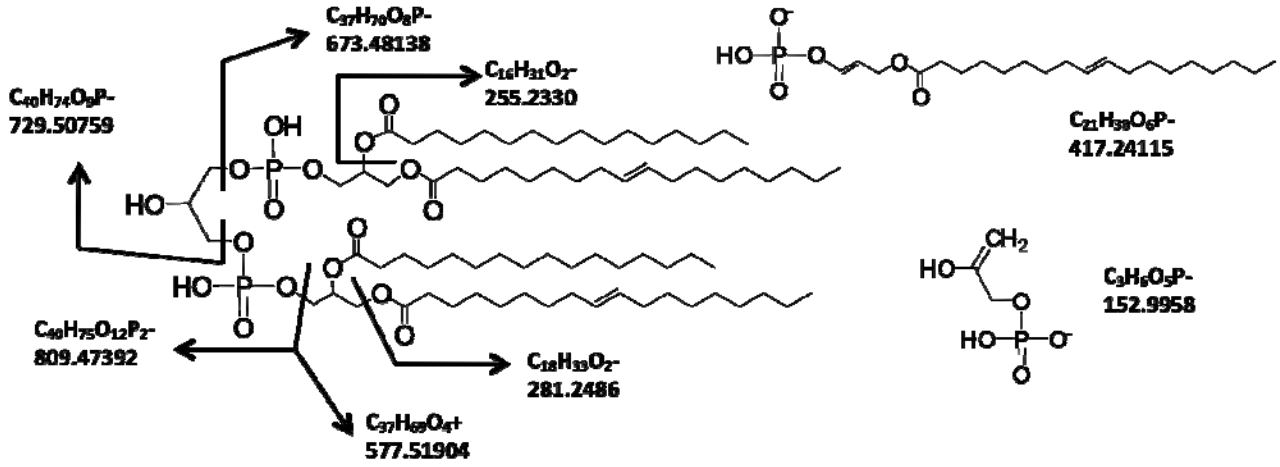
785.6211	4.0	menaquinones(45:8)H-
916.5681	5.3	mycobactins(19:0)CH3COO- mycobactins(20:0)HCOO-
898.5986	5.7	mycobactins(22:0)H- dideoxymycobactins(20:0)CH3COO- dideoxymycobactins(21:0)HCOO-
810.5420	7.1	dideoxymycobactins(18:0)H-
910.5847	7.5	dideoxymycobactins(21:1)CH3COO-dideoxymycobactins(22:1)HCOO-
864.5920	6.0	dideoxymycobactins(22:1)H-
942.6228	10.0	monodeoxymycobactins(22:0)CH3COO-
679.4927	24.5	mycoketidesmannosyl phospho(30:0)H-
707.5215	24.4	mycoketidesmannosyl phospho(32:0)H-
909.6375	22.3	decaprenylphosphoribose(50:10)H-
1039.6591	22.5	diacylated sulfoglycolipids(41:0)H-
1065.6678	24.1	diacylated sulfoglycolipids(43:0)H-
1067.6906	22.4	diacylated sulfoglycolipids(43:0)H-
1109.7371	22.6	diacylated sulfoglycolipids(46:0)H-
1107.7587	22.5	diacylated sulfoglycolipids(47:0)H-
1123.7525	22.7	diacylated sulfoglycolipids(47:0)H-
1149.7716	22.6	diacylated sulfoglycolipids(49:0)H-
1151.7839	22.6	diacylated sulfoglycolipids(49:0)H-
1149.8023	22.3	diacylated sulfoglycolipids(50:0)H-
1165.7998	22.7	diacylated sulfoglycolipids(50:0)H-
1191.8188	22.5	diacylated sulfoglycolipids(52:0)H-
1193.8308	22.6	diacylated sulfoglycolipids(52:0)H-
1191.8474	22.2	diacylated sulfoglycolipids(53:0)H-
1207.8460	22.6	diacylated sulfoglycolipids(53:0)H-
1233.8624	22.5	diacylated sulfoglycolipids(55:0)H-
1235.8780	22.5	diacylated sulfoglycolipids(55:0)H-
1233.8961	22.1	diacylated sulfoglycolipids(56:0)H-
1249.8937	22.5	diacylated sulfoglycolipids(56:0)H-
1275.9085	22.4	diacylated sulfoglycolipids(58:0)H-
1277.9264	22.4	diacylated sulfoglycolipids(58:0)H-
1275.9406	22.0	diacylated sulfoglycolipids(59:0)H-
1291.9415	22.4	diacylated sulfoglycolipids(59:0)H-
1303.9348	22.3	diacylated sulfoglycolipids(60:0)H-
1317.9512	22.3	diacylated sulfoglycolipids(61:0)H-
1319.9722	22.3	diacylated sulfoglycolipids(61:0)H-
1333.9834	22.3	diacylated sulfoglycolipids(62:0)H-
1359.9984	22.2	diacylated sulfoglycolipids(64:0)H-
1362.0192	22.1	diacylated sulfoglycolipids(64:0)H-
1376.0336	22.1	diacylated sulfoglycolipids(65:0)H-
1404.0638	22.0	diacylated sulfoglycolipids(67:0)H-
721.5011	23.3	phosphatidylglycerols(32:0)H-
719.4862	23.4	phosphatidylglycerols(32:1)H-
717.4712	23.5	phosphatidylglycerols(32:2)H-
749.5302	23.1	phosphatidylglycerols(34:0)H-
747.5161	23.2	phosphatidylglycerols(34:1)H-
761.5331	23.1	phosphatidylglycerols(35:1)H-
691.4570	23.5	phosphatidylglycerols(30:1)H-
735.5165	23.2	phosphatidylglycerols(33:0)H-
745.5018	23.3	phosphatidylglycerols(34:2)H-
777.5640	23.0	phosphatidylglycerols(36:0)H-
775.5492	23.0	phosphatidylglycerols(36:1)H-
773.5330	23.1	phosphatidylglycerols(36:2)H-
647.4654	24.1	phosphatidic acids(32:0)H-
675.4969	24.1	phosphatidic acids(34:0)H-
673.4814	24.1	phosphatidic acids(34:1)H-
671.4633	24.1	phosphatidic acids(34:2)H-
703.5280	24.1	phosphatidic acids(36:0)H-
701.5075	24.1	phosphatidic acids(36:1)H-
662.4771	26.2	phosphatidylethanolamines(30:0)H-
660.4602	26.3	phosphatidylethanolamines(30:1)H-
690.5093	26.0	phosphatidylethanolamines(32:0)H-
686.4764	26.3	phosphatidylethanolamines(32:2)H-
704.5304	24.1	phosphatidylethanolamines(33:0)H-
704.5248	25.9	phosphatidylethanolamines(33:0)H-

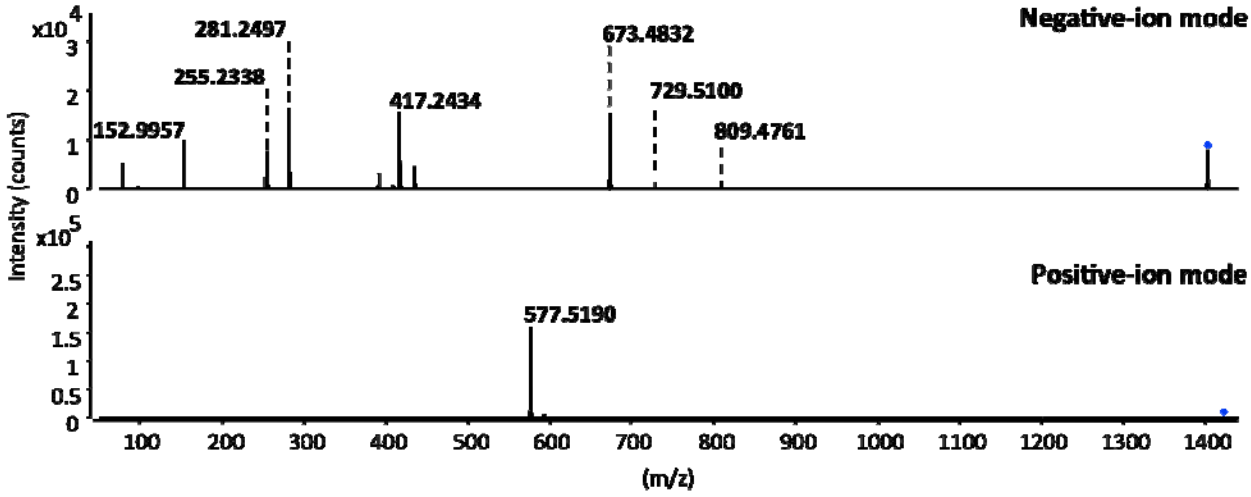
718.5386	22.1	phosphatidylethanolamines(34:0)H-
718.5413	25.8	phosphatidylethanolamines(34:0)H-
716.5252	25.9	phosphatidylethanolamines(34:1)H-
714.5088	26.0	phosphatidylethanolamines(34:2)H-
732.5575	25.7	phosphatidylethanolamines(35:0)H-
732.5556	22.0	phosphatidylethanolamines(35:0)H-
730.5407	25.8	phosphatidylethanolamines(35:1)H-
746.5726	25.6	phosphatidylethanolamines(36:0)H-
744.5568	25.6	phosphatidylethanolamines(36:1)H-
742.5406	25.8	phosphatidylethanolamines(36:2)H-
760.5877	25.5	phosphatidylethanolamines(37:0)H-
758.5727	25.6	phosphatidylethanolamines(37:1)H-
774.6031	25.4	phosphatidylethanolamines(38:0)H-
772.5822	25.5	phosphatidylethanolamines(38:1)H-
802.6310	25.3	phosphatidylethanolamines(40:0)H-
830.6626	25.2	phosphatidylethanolamines(42:0)H-
1382.0222	26.0	phosphatidylethanolamines dimer(32:0)H-
1438.0864	25.8	phosphatidylethanolamines dimer(34:0)H-
1466.1190	25.7	phosphatidylethanolamines dimer(35:0)H-
1494.1354	25.6	phosphatidylethanolamines dimer(36:0)H-
1323.9264	25.2	cardiolipins(62:0)H-
1321.9141	25.2	cardiolipins(62:1)H-
1319.8034	25.2	cardiolipins(62:2)H-
1317.8806	25.3	cardiolipins(62:3)H-
1335.9275	25.2	cardiolipins(63:1)H-
1351.9547	25.2	cardiolipins(64:0)H-
1349.9430	25.2	cardiolipins(64:1)H-
1347.9317	25.2	cardiolipins(64:2)H-
1345.9169	25.2	cardiolipins(64:3)H-
1343.9013	25.2	cardiolipins(64:4)H-
1365.9672	25.1	cardiolipins(65:0)H-
1363.9629	25.1	cardiolipins(65:1)H-
1361.9465	25.2	cardiolipins(65:2)H-
1359.9323	25.2	cardiolipins(65:3)H-
1357.9111	25.2	cardiolipins(65:4)H-
1379.9836	25.1	cardiolipins(66:0)H-
1380.0044	26.1	cardiolipins(66:0)H-
1377.9741	25.1	cardiolipins(66:1)H-
1375.9631	25.1	cardiolipins(66:2)H-
1373.9483	25.2	cardiolipins(66:3)H- phosphatidylethanolamines dimer(32:2)H-
1371.9327	25.2	cardiolipins(66:4)H-
1394.0006	25.0	cardiolipins(67:0)H-
1391.9909	25.0	cardiolipins(67:1)H-
1389.9782	25.1	cardiolipins(67:2)H-
1387.9626	25.1	cardiolipins(67:3)H-
1385.9465	25.2	cardiolipins(67:4)H-
1408.0383	25.9	cardiolipins(68:0)H-
1406.0030	24.9	cardiolipins(68:1)H-
1403.9941	25.0	cardiolipins(68:2)H-
1401.9800	25.0	cardiolipins(68:3)H-
1399.9645	25.1	cardiolipins(68:4)H-
1422.0488	25.9	cardiolipins(69:0)H-
1422.0323	24.8	cardiolipins(68:0)H-
1420.0243	24.8	cardiolipins(69:1)H-
1418.0094	24.9	cardiolipins(69:2)H-
1415.9936	24.9	cardiolipins(69:3)H-
1413.9683	25.1	cardiolipins(69:4)H-
1436.0515	24.8	cardiolipins(70:0)H-
1436.0704	25.8	cardiolipins(70:0)H-
1434.0344	24.8	cardiolipins(70:1)H-
1434.0502	25.9	cardiolipins(70:1)H- phosphatidylethanolamines dimer(35:1)H- phosphatidylethanolamines dimer(34:1)H-
1432.0219	24.8	cardiolipins(70:2)H-
1430.0096	24.8	cardiolipins(70:3)H- phosphatidylethanolamines dimer(34:2)H-
1427.9935	24.9	cardiolipins(70:4)H-

1450.0864	25.8	cardiolipins(71:0)H-
1448.0506	24.8	cardiolipins(71:1)H-
1446.0387	24.8	cardiolipins(71:2)H-
1444.0192	24.8	cardiolipins(71:3)H-
1464.0970	25.7	cardiolipins(72:0)H-
1462.0648	24.8	cardiolipins(72:1)H-
1462.0730	25.8	cardiolipins(72:1)H- phosphatidylethanolamines dimer(35:1)H- phosphatidylethanolamines dimer(35:1)H-
1460.0457	24.8	cardiolipins(72:2)H-
1460.0656	25.8	cardiolipins(72:2)H-
1458.0296	24.8	cardiolipins(72:3)H-
1458.0498	25.8	cardiolipins(72:3)H- phosphatidylethanolamines dimer(35:2)H-
1456.0177	24.8	cardiolipins(72:4)H-
1478.1151	25.6	cardiolipins(73:0)H-
1474.0755	25.7	cardiolipins(73:2)H-
1472.0649	25.7	cardiolipins(73:3)H-
1488.0965	25.6	cardiolipins(74:2)H-
1486.0795	25.7	cardiolipins(74:3)H- phosphatidylethanolamines dimer(36:2)H-
1502.1111	25.5	cardiolipins(75:2)H-
1544.1393	24.7	cardiolipins(78:2)H-
1652.1321	25.3	diacyl phosphatidylinositol dimannosides(67:0)H-
1680.1595	25.3	diacyl phosphatidylinositol dimannosides(69:0)H-
1694.1785	25.2	diacyl phosphatidylinositol dimannosides(70:0)H-
781.4873	27.2	phosphatidylinositols(30:0)H-
807.5019	27.0	phosphatidylinositols(32:1)H-
823.5344	26.8	phosphatidylinositols(33:0)H-
837.5496	26.7	phosphatidylinositols(34:0)H-
835.5344	26.8	phosphatidylinositols(34:1)H-
833.5182	27.0	phosphatidylinositols(34:2)H-
849.5496	26.7	phosphatidylinositols(35:1)H-
865.5805	26.4	phosphatidylinositols(36:0)H-
861.5502	26.7	phosphatidylinositols(36:2)H-
879.5961	26.3	phosphatidylinositols(37:0)H-
877.5801	26.4	phosphatidylinositols(37:1)H-
893.6078	26.3	phosphatidylinositols(38:0)H-
1413.8006	27.9	monoacyl phosphatidylinositol dimannosides(51:0)H-
1441.9294	26.8	monoacyl phosphatidylinositol dimannosides(53:0)H-
424.2492	31.6	lyso phosphatidylethanolamines(14:0)H-
452.2801	30.4	lyso phosphatidylethanolamines(16:0)H-
452.2809	31.1	lyso phosphatidylethanolamines(16:0)H-
450.2644	31.5	lyso phosphatidylethanolamines(16:1)H-
480.3114	30.7	lyso phosphatidylethanolamines(18:0)H-
480.3119	30.0	lyso phosphatidylethanolamines(18:0)H-
478.2961	31.1	lyso phosphatidylethanolamines(18:1)H-
494.3268	30.6	lyso phosphatidylethanolamines(19:0)H-
508.3413	30.4	lyso phosphatidylethanolamines(20:0)H-

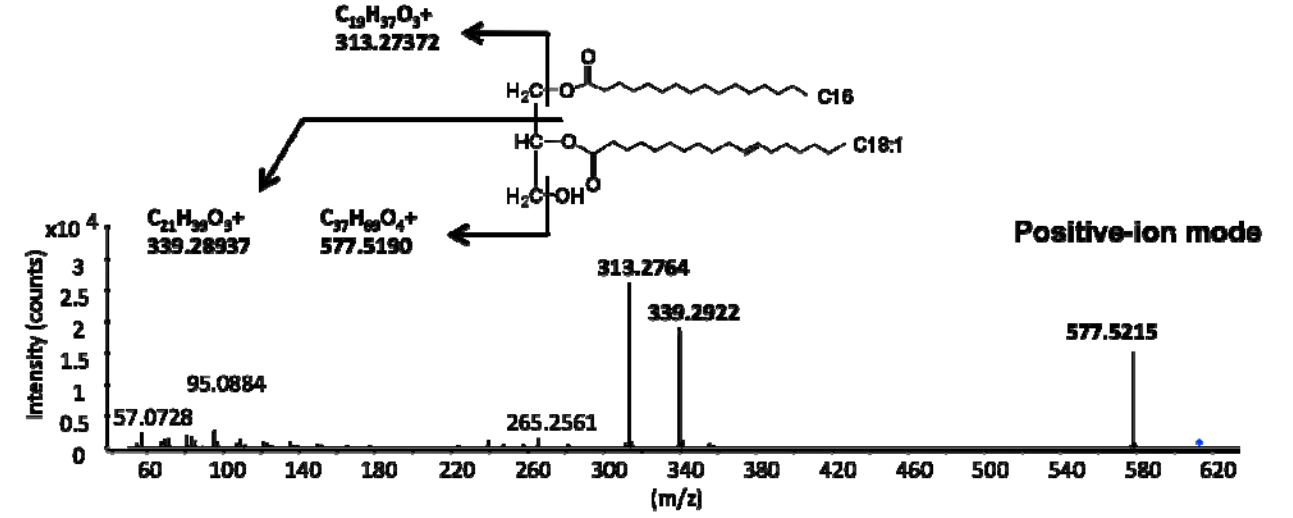
Figure S4, related to Figure 4 (continued)

Cardiolipin	M-H-, $C_{77}H_{145}O_{17}P_2$- 1403.9962	M+NH_4+, $C_{77}H_{150}NO_{17}P_2$+, 1423.03735

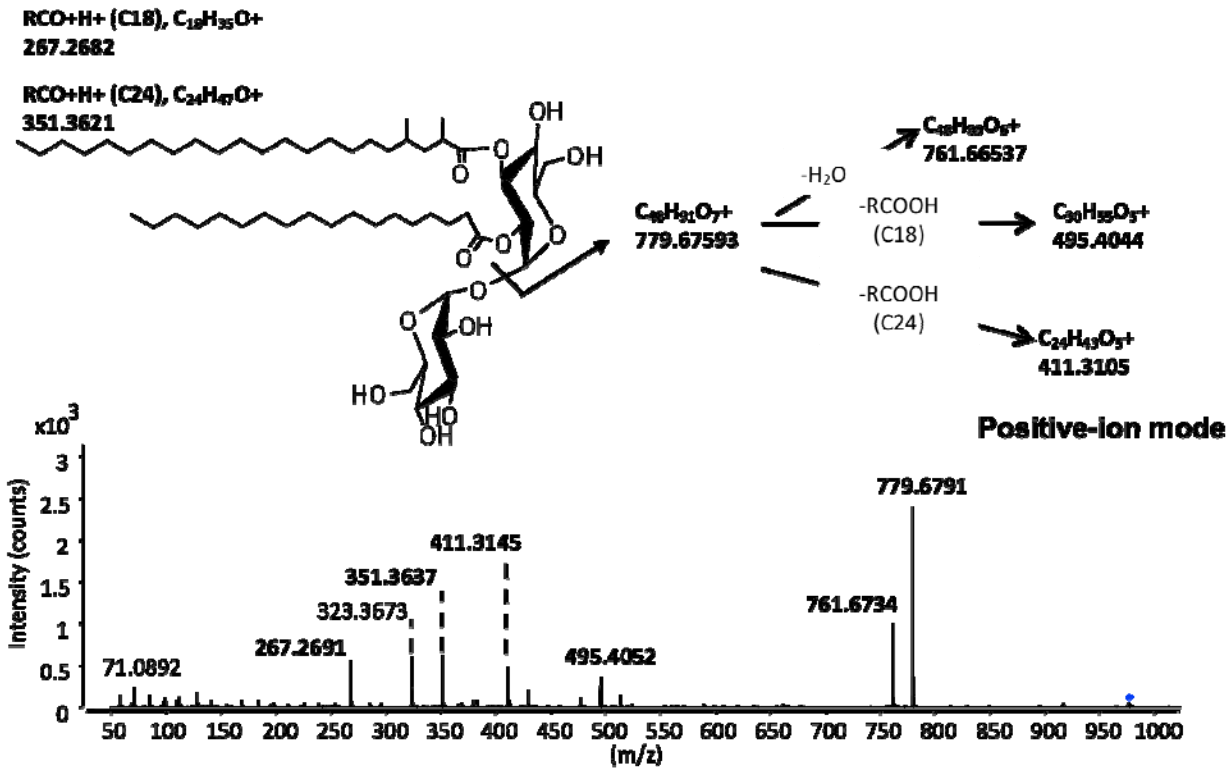




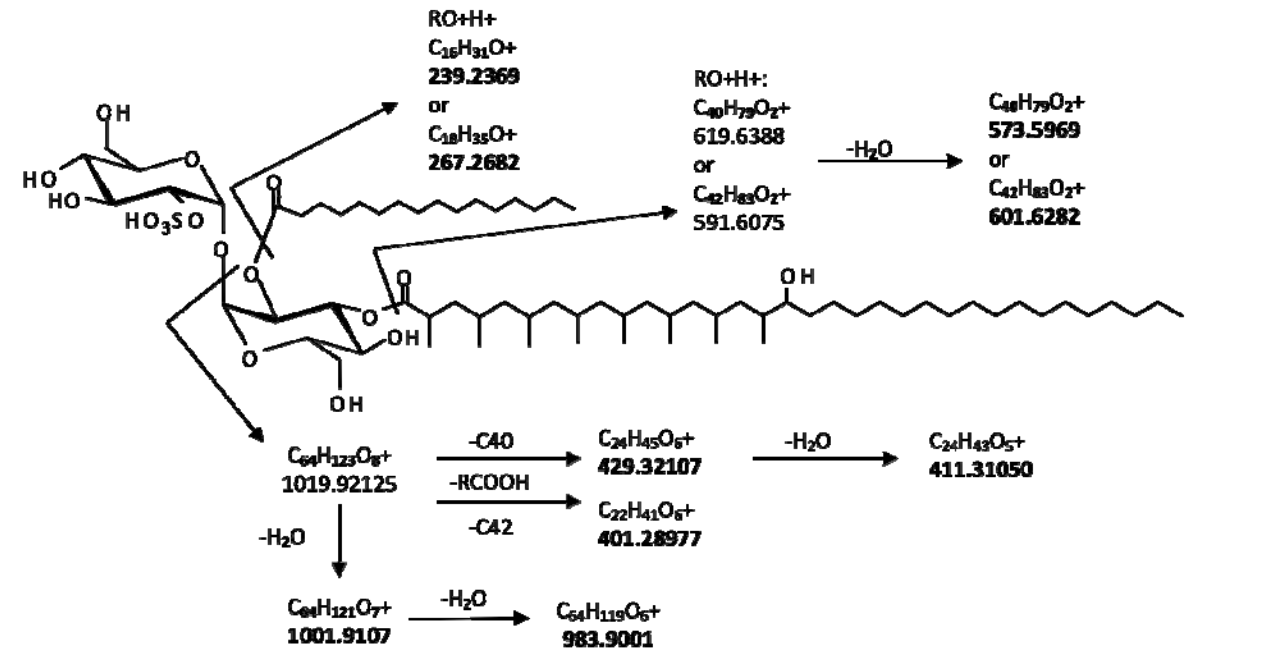
Diacylated glycerol	M+NH_4+, $C_{37}H_{74}NO_5$+ 612.5562

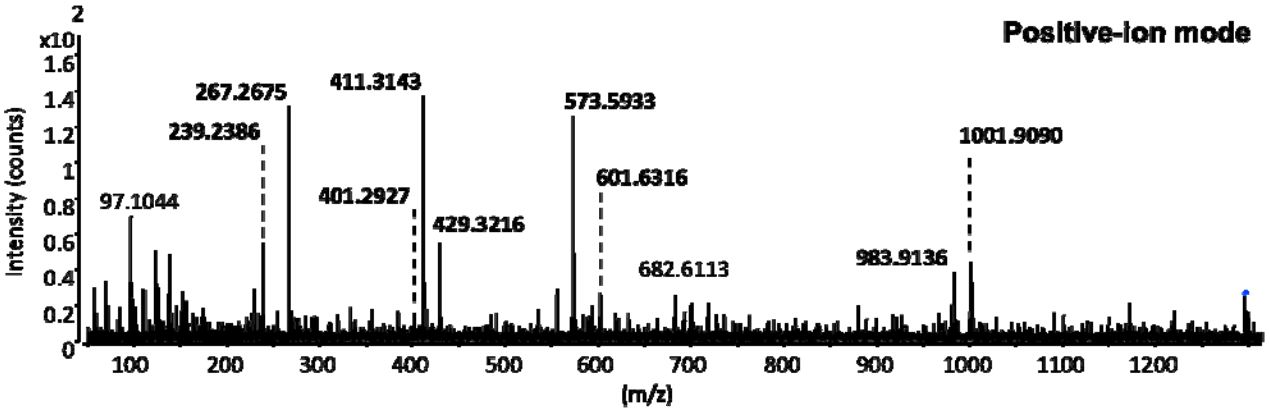


Diacylated trehalose	$M+NH_4+$, $C_{54}H_{106}NO_{13}+$ 976.76587

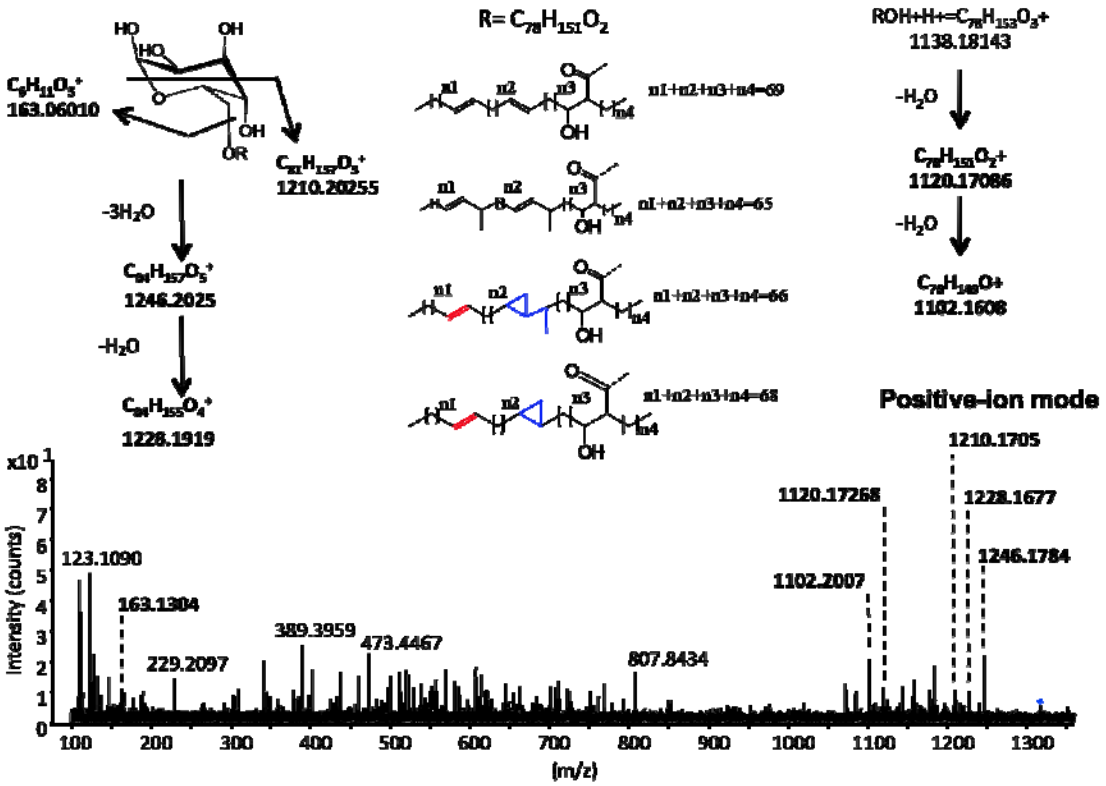


Diacylated sulfoglycolipids (C16, C42 or C18, C40)	$M+NH_4+$, $C_{70}H_{138}NO_{17}S+$ 1296.96855

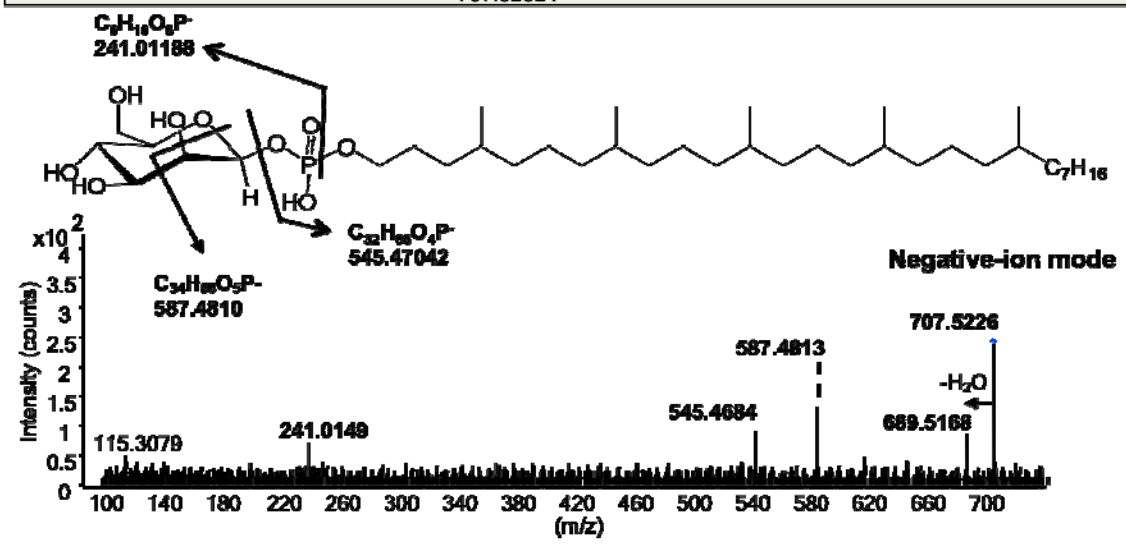




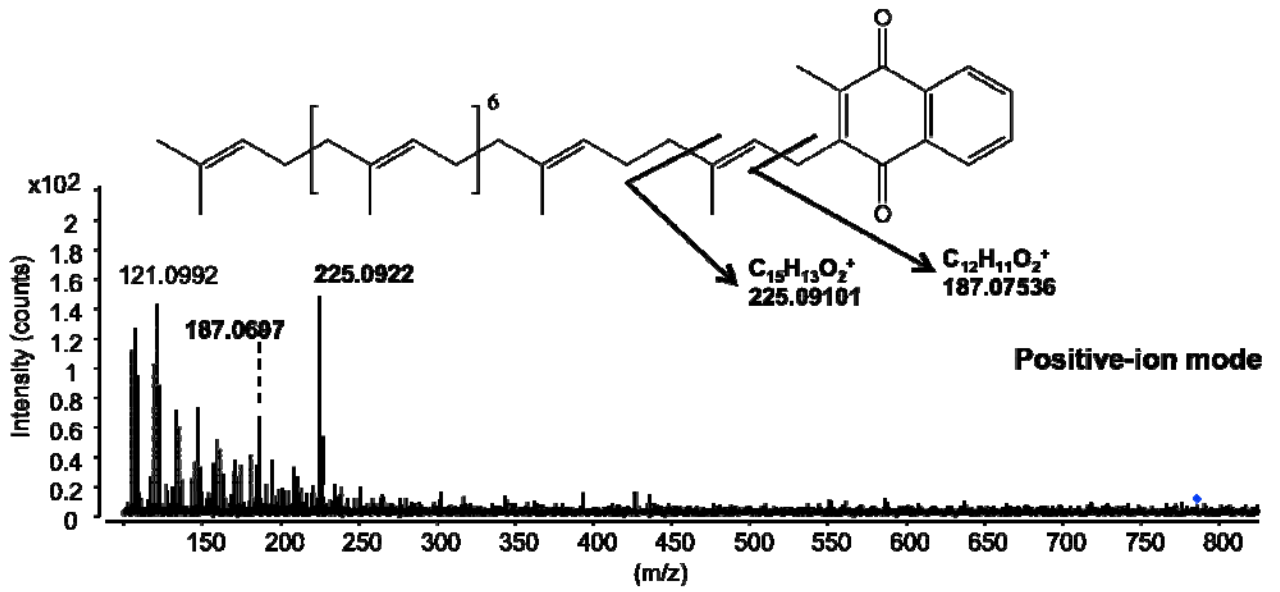
Glucose monomycolate (C78 alpha)



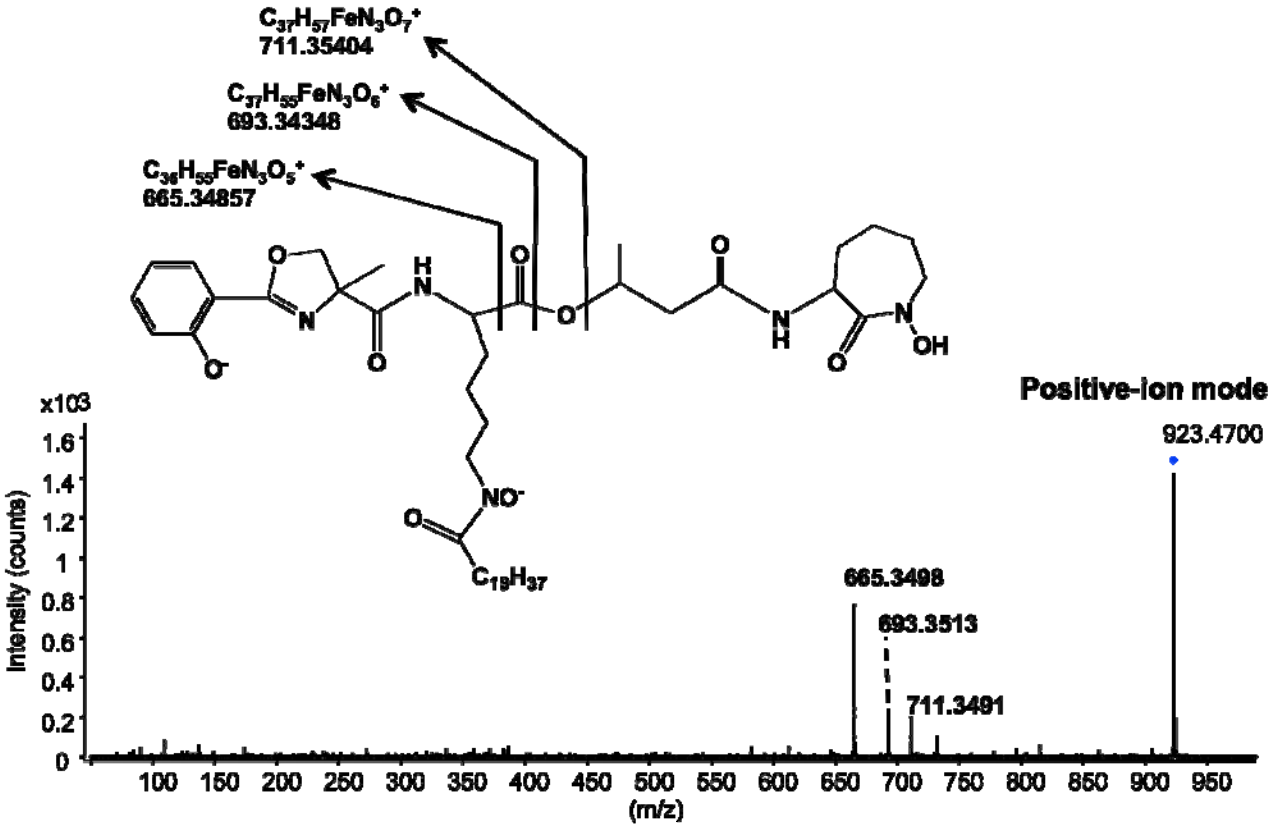
Mannosyl phosphomycoketide M-H- , $C_{38}H_{76}O_9P^-$ 707.52324



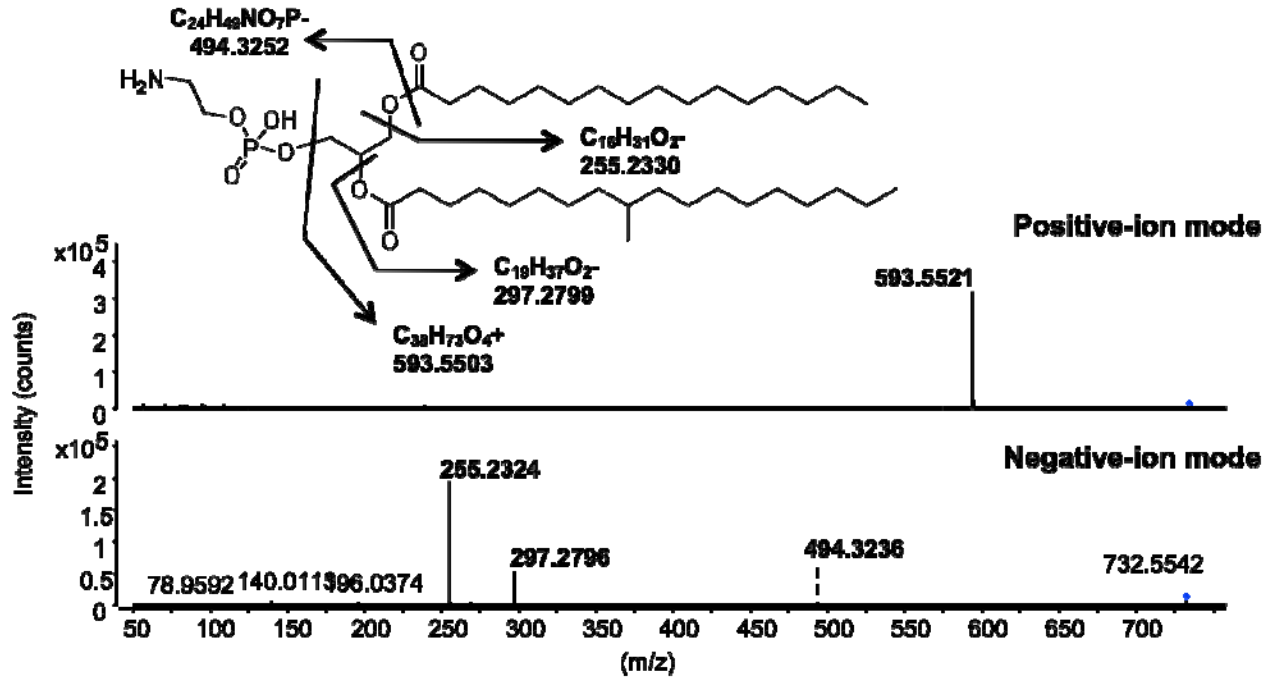
Menaquinone	M+H, $C_{56}H_{81}O_2^+$ 785.62311



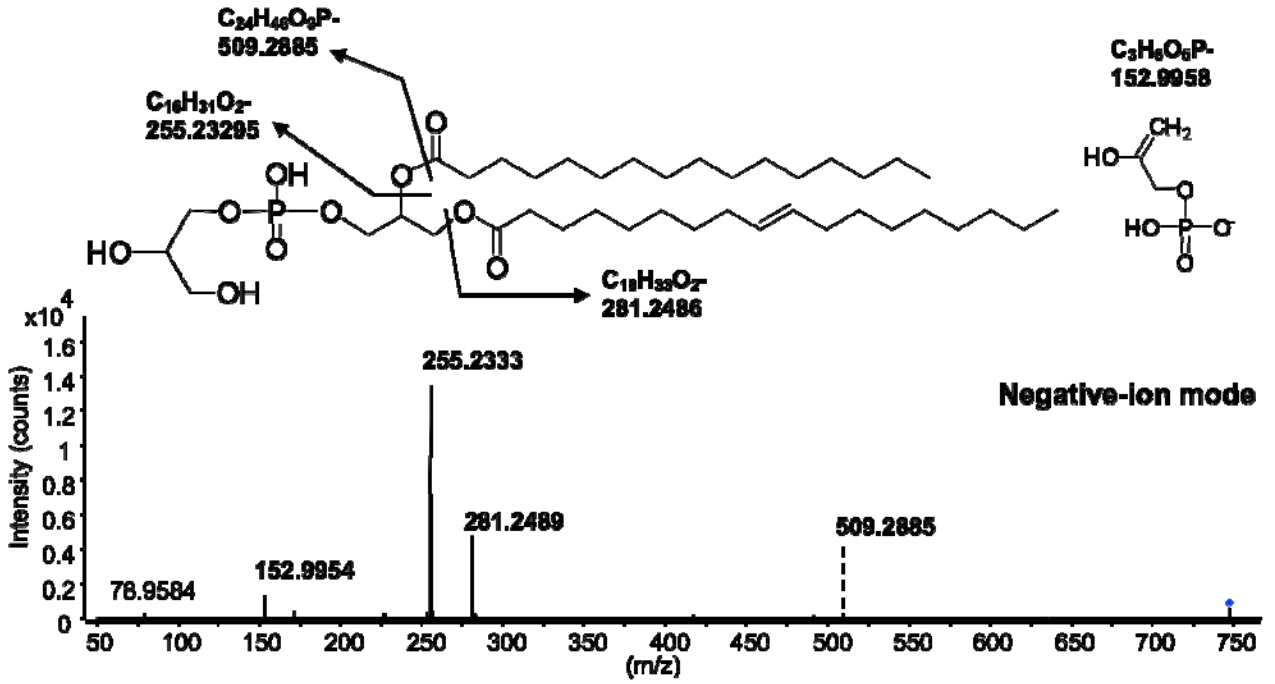
Mycobactin (C20:0)	M-2H+Fe^{3+}, $C_{47}H_{73}FeN_5O_{10}^+$ 923.4701



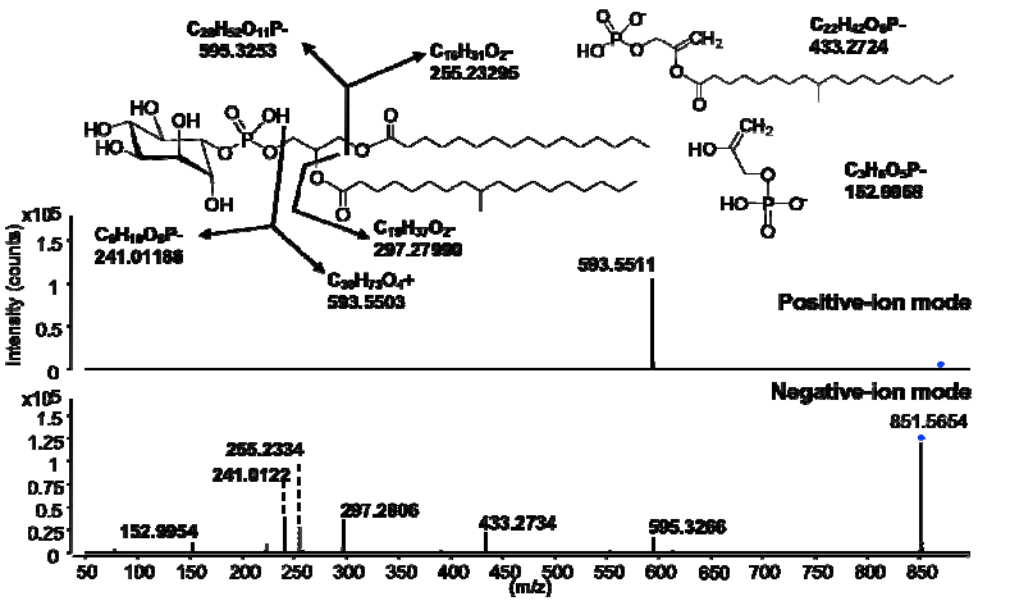
Phosphatidyl ethanolamine	M+H+, $C_{40}H_{81}NO_8P$+ 734.5694	M-H-, $C_{40}H_{79}NO_8P$- 732.55488



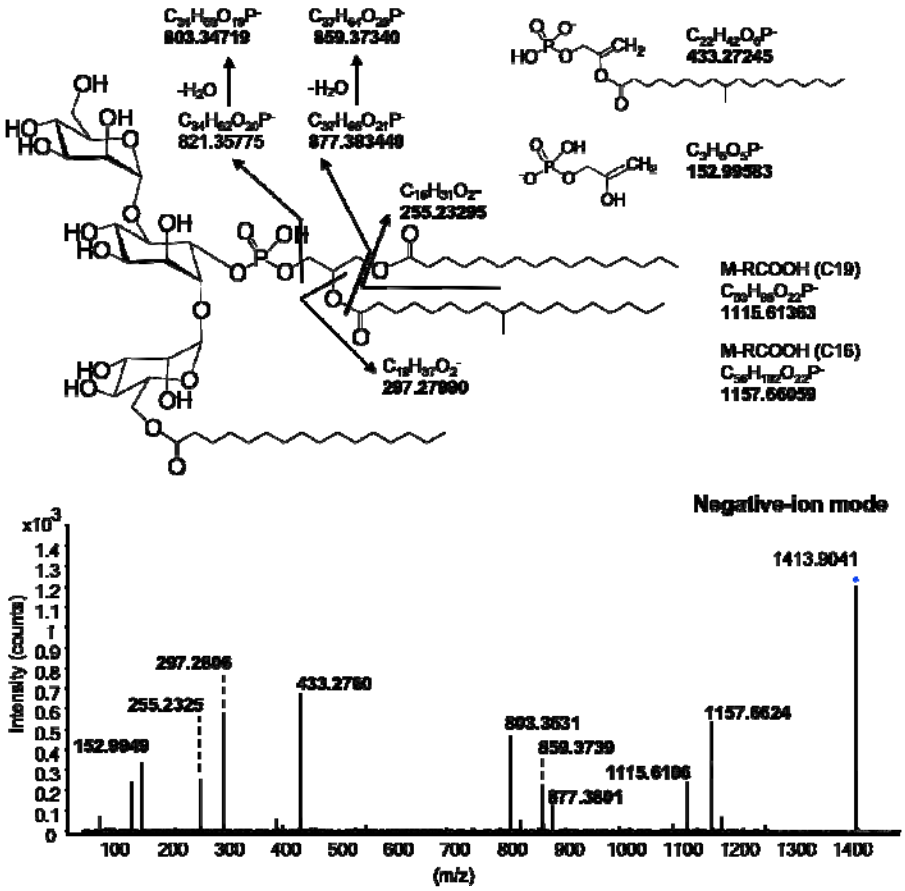
Phosphatidyl glycerol	M-H-, $C_{40}H_{76}O_{10}P$- 747.5182



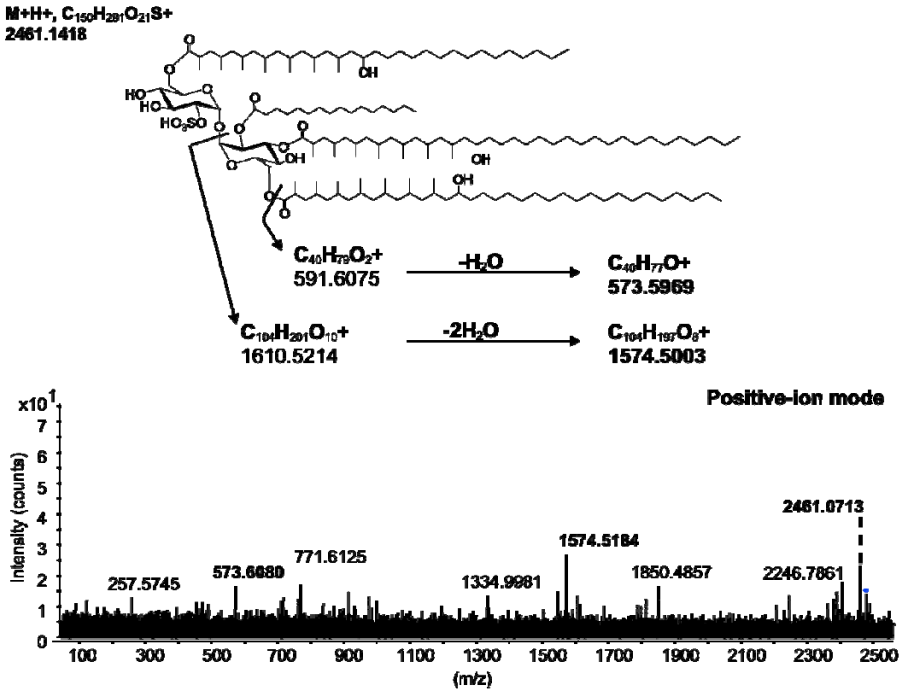
Phosphatidyl inositol	M+NH4+, $C_{44}H_{89}NO_{13}P^+$ 870.6066	M-H-, $C_{44}H_{84}O_{13}P^-$ 851.5655



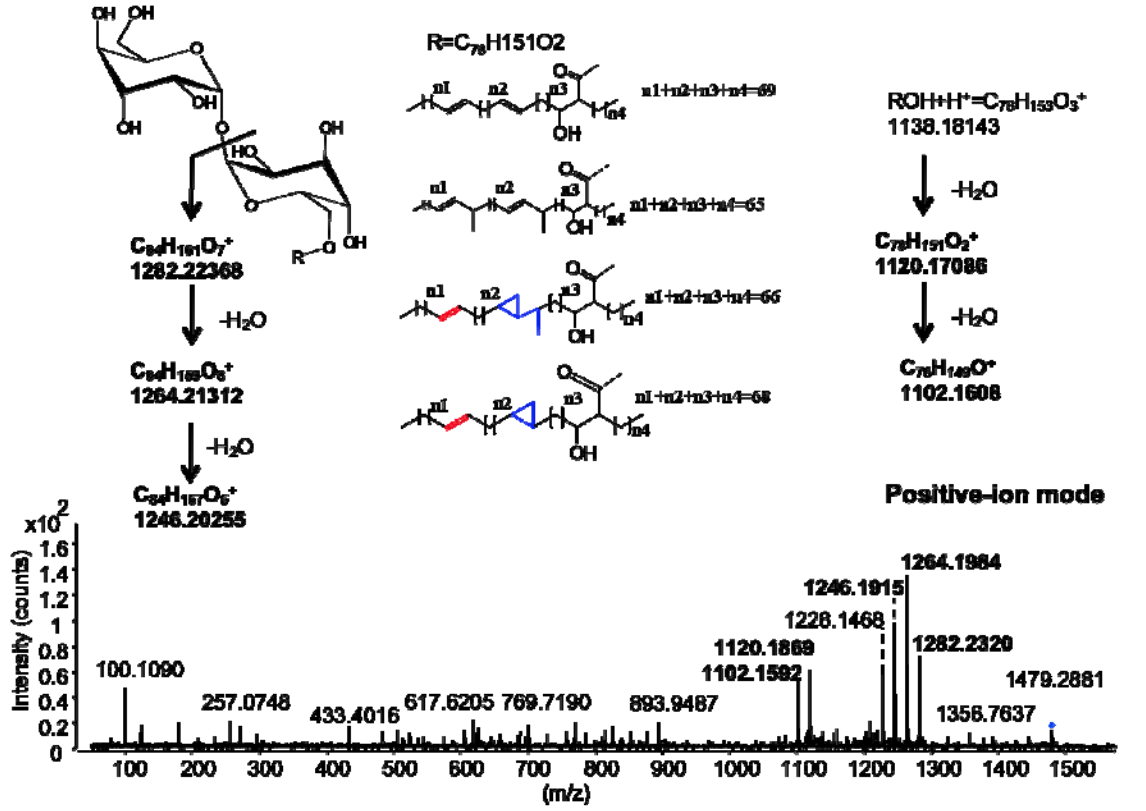
PIM_2Ac_1	M-H-, $C_{72}H_{134}O_{24}P^-$ 1413.90082



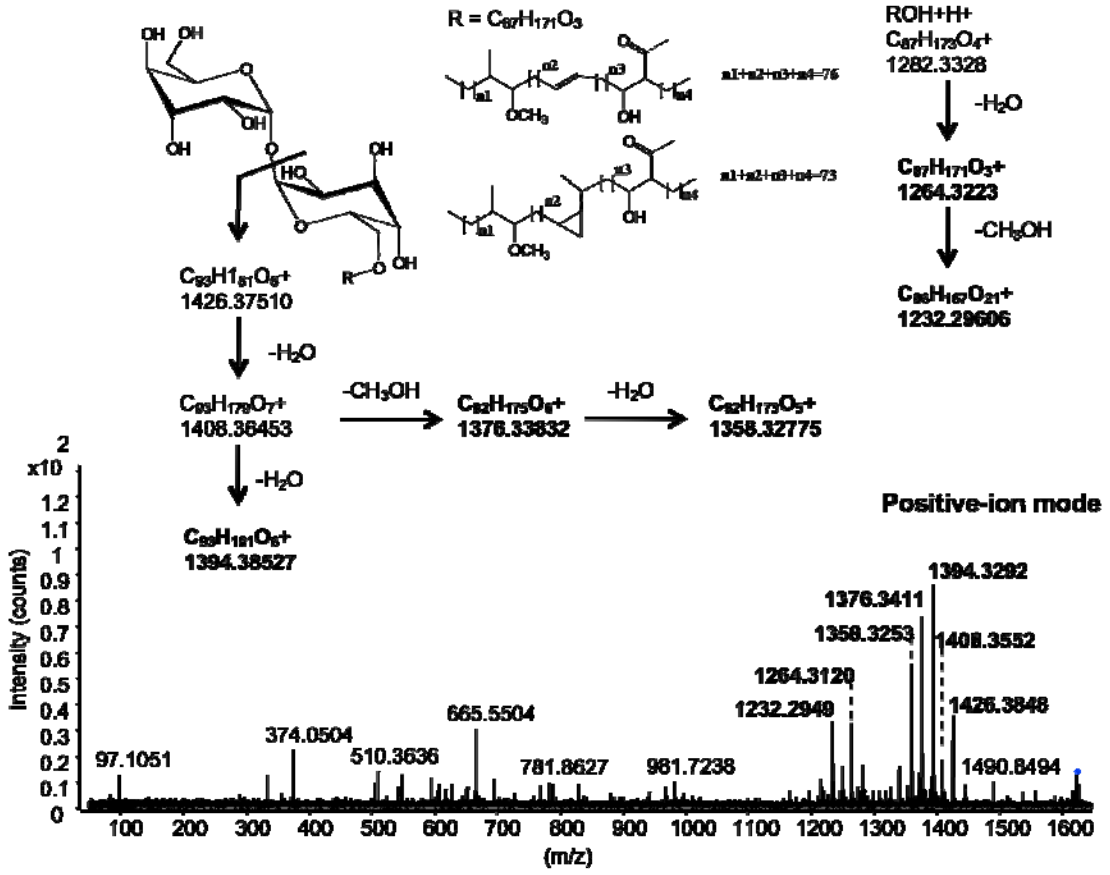
Tetraacylated sulfoglycolipids (C16, C38, C40, C42)	$M+NH_4^+$, $C_{150}H_{294}NO_{21}S^+$ 2478.1684



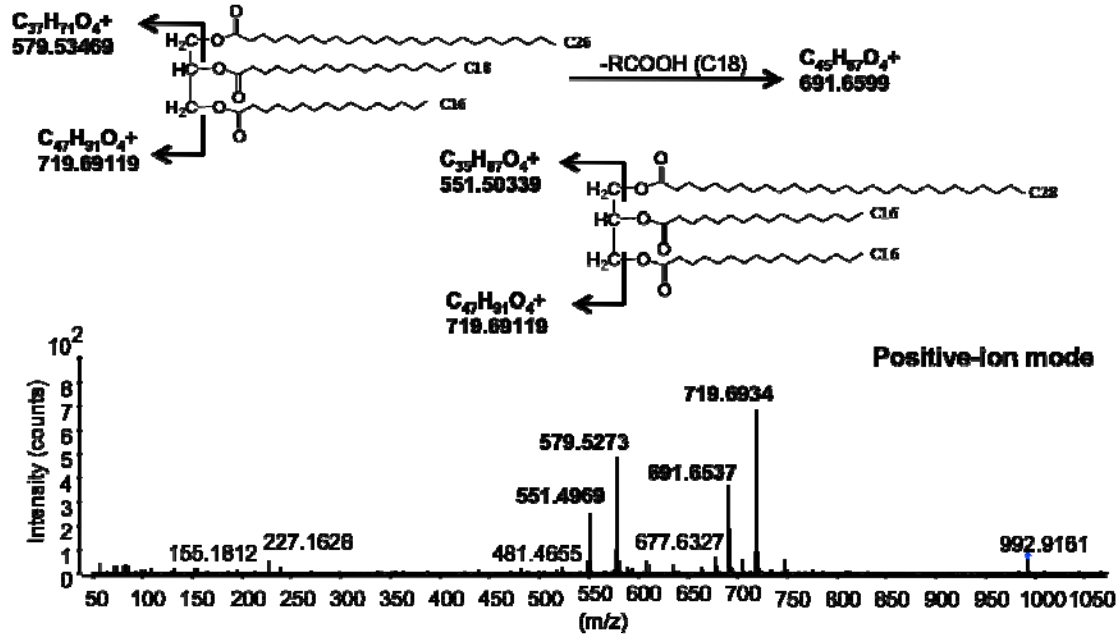
Trehalose Monomycolate (C78 alpha)	$M+NH_4^+$, $C_{90}H_{176}NO_{13}^+$ 1479.3136



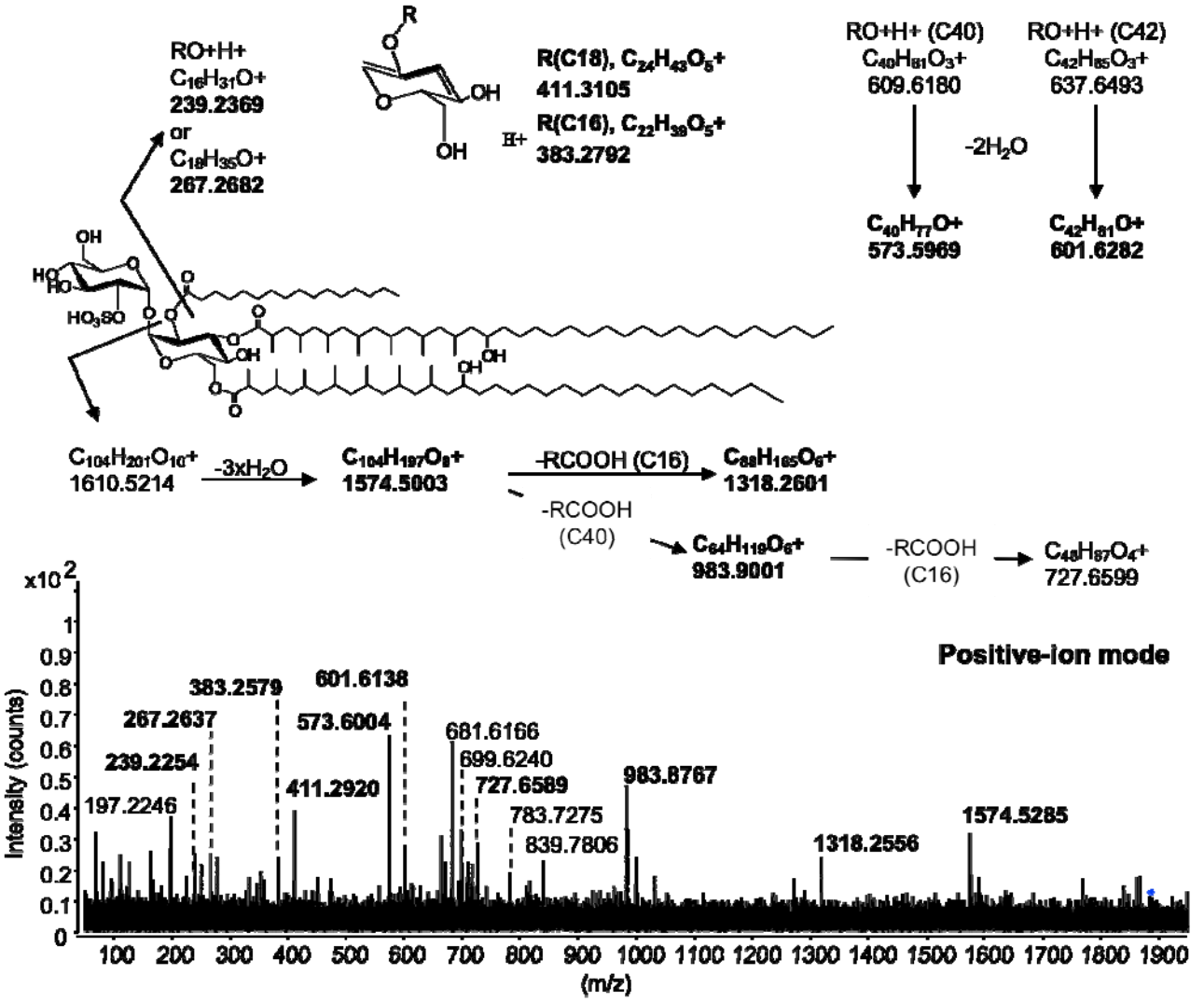
Trehalose Monomycolate, C87 methoxy



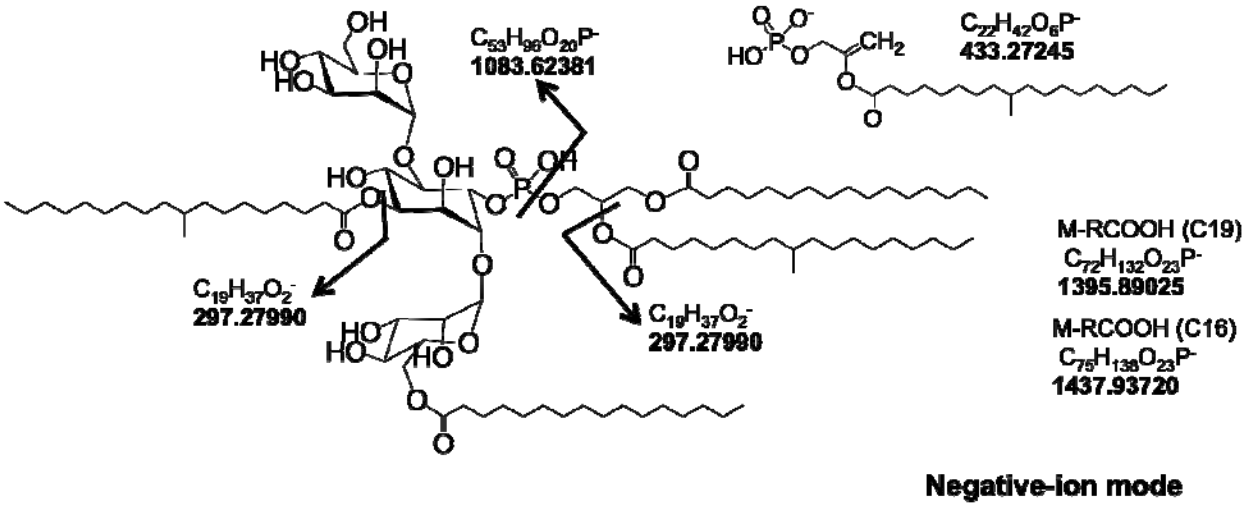
Triacylated glycerol $M+NH_4^+$, $C_{63}H_{126}NO_6^+$ 992.9580



Triacylated sulfoglycolipids (C16, C40, C42 or C18, 2C40)	$M+NH_4+$, $C_{110}H_{216}NO_{19}S+$ 1887.5682



PIM_2Ac_2 (2C16, 2C19)	M-H-, $C_{91}H_{170}O_{25}P^-$ 1694.17743



Negative-ion mode

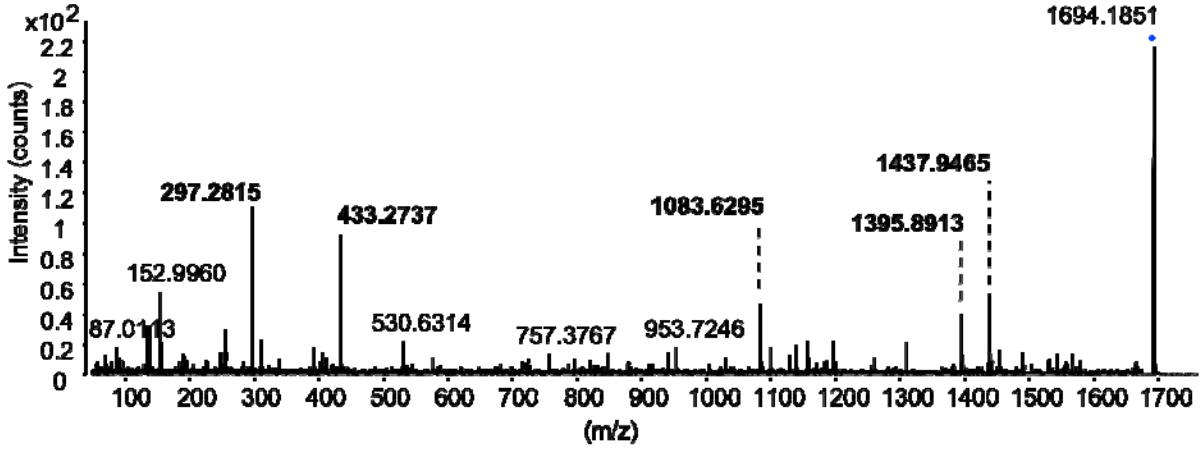


Figure S5, related to Figure 5. The *MycoMap* database. All detected alkylforms of mycobacterial lipid families assigned by prior collisional experiments are listed in *MycoMap* database indicating the detected adducts in specific ionization-mode and their *m/z*, mass accuracy compared to calculated *m/z* expected for the respective adduct (amu) as well as the observed retention time for the lipid group. Retention time values are given for one dataset, but actual values can vary up to 60 secondes variance based on user and column dependent factors. For simplicity only one type of adduct is listed per alkylform and detected *m/z* and naturally negative lipids are listed for the negative-ion mode, although they are also detected in positive-ion mode as protonated or ammoniated adducts. Lipid nomenclature is described in the legend of the **Figure S1**. (NA: non applicable).

MycoMap - 30 lipid families, 318 molecules

Category/ Main Class / Subclass	Family	Formula	Detected m/z	Ion-mode/Adduct	Calculated m/z	Δm (amu)	RT (min)
Polyketides/ Linear polyketides/ NA	phthiocerol dimycocerosate PDIM A/A'	C87H172O5	1315.3468	pos/[M+NH4]+	1315.3543	0.0075	3.6
		C88H174O5	1329.3640	pos/[M+NH4]+	1329.3699	0.0059	
		C89H176O5	1343.3891	pos/[M+NH4]+	1343.3856	0.0035	
		C90H178O5	1357.3980	pos/[M+NH4]+	1357.4012	0.0032	
		C91H180O5	1371.4137	pos/[M+NH4]+	1371.4169	0.0032	
		C92H182O5	1385.4330	pos/[M+NH4]+	1385.4325	0.0005	
		C93H184O5	1399.4461	pos/[M+NH4]+	1399.4482	0.0021	
		C94H186O5	1413.4643	pos/[M+NH4]+	1413.4638	0.0005	
		C95H188O5	1427.4706	pos/[M+NH4]+	1427.4795	0.0089	
		C96H190O5	1441.4888	pos/[M+NH4]+	1441.4951	0.0063	
		C97H192O5	1455.5082	pos/[M+NH4]+	1455.5108	0.0026	
		C98H194O5	1469.5251	pos/[M+NH4]+	1469.5264	0.0013	
		C99H196O5	1483.5338	pos/[M+NH4]+	1483.5421	0.0083	
		C100H198O5	1497.5559	pos/[M+NH4]+	1497.5577	0.0018	
		C101H200O5	1511.5544	pos/[M+NH4]+	1511.5734	0.0190	
		C102H202O5	1525.5703	pos/[M+NH4]+	1525.5891	0.0188	
	phthiocerol dimycocerosate PDIM B	C87H170O5	1313.3370	pos/[M+NH4]+	1313.3387	0.0017	
		C88H172O5	1327.3547	pos/[M+NH4]+	1327.3543	0.0004	
		C89H174O5	1341.3696	pos/[M+NH4]+	1341.3700	0.0004	
		C90H176O5	1355.3854	pos/[M+NH4]+	1355.3856	0.0002	
		C91H178O5	1369.4017	pos/[M+NH4]+	1369.4013	0.0004	
		C92H180O5	1383.4162	pos/[M+NH4]+	1383.4169	0.0007	
		C93H182O5	1397.4325	pos/[M+NH4]+	1397.4326	0.0001	
		C94H184O5	1411.4483	pos/[M+NH4]+	1411.4482	0.0001	
		C95H186O5	1425.4487	pos/[M+NH4]+	1425.4639	0.0152	
		C96H188O5	1439.4791	pos/[M+NH4]+	1439.4795	0.0004	
		C97H190O5	1453.4928	pos/[M+NH4]+	1453.4952	0.0024	
		C98H192O5	1467.5050	pos/[M+NH4]+	1467.5108	0.0058	
		C99H194O5	1481.5243	pos/[M+NH4]+	1481.5265	0.0022	
		C100H196O5	1495.5490	pos/[M+NH4]+	1495.5421	0.0069	
		C101H198O5	1509.5480	pos/[M+NH4]+	1509.5578	0.0098	
		C102H200O5	1523.5480	pos/[M+NH4]+	1523.5734	0.0254	
Fatty acyls/ Fatty acids and Conjugates/ Mycolic acids	methoxy mycolic acids	C81H160O4	1196.2201	neg/[M-H]-	1196.2244	0.0043	3.6-3.7
		C82H162O4	1210.2227	neg/[M-H]-	1210.2400	0.0173	
		C83H164O4	1224.2518	neg/[M-H]-	1224.2557	0.0039	
		C84H166O4	1238.2612	neg/[M-H]-	1238.2713	0.0101	
		C85H168O4	1252.2830	neg/[M-H]-	1252.2870	0.0040	
		C87H172O4	1280.3137	neg/[M-H]-	1280.3183	0.0046	
		C88H174O4	1294.3186	neg/[M-H]-	1294.3339	0.0153	

Glycerolipids/ Triradylglycerols/ Triacylglycerols	triacylglycerols	C51H98O6	824.7661	pos/[M+NH4]+	824.7706	0.0045	3.7
		C53H100O6	850.7837	pos/[M+NH4]+	850.7864	0.0027	
		C54H102O6	864.7990	pos/[M+NH4]+	864.8020	0.0030	
		C55H104O6	878.8131	pos/[M+NH4]+	878.8177	0.0046	
		C56H108O6	894.8393	pos/[M+NH4]+	894.8488	0.0095	
		C57H108O6	906.8481	pos/[M+NH4]+	906.8490	0.0009	
		C57H110O6	908.8631	pos/[M+NH4]+	908.8645	0.0014	
		C58H112O6	922.8694	pos/[M+NH4]+	922.8801	0.0107	
		C59H112O6	934.8791	pos/[M+NH4]+	934.8803	0.0012	
		C60H116O6	950.9182	pos/[M+NH4]+	950.9114	0.0068	
		C61H116O6	962.9068	pos/[M+NH4]+	962.9116	0.0028	
		C61H118O6	964.9266	pos/[M+NH4]+	964.9271	0.0005	
		C62H120O6	978.9305	pos/[M+NH4]+	978.9427	0.0122	
		C63H122O6	992.9576	pos/[M+NH4]+	992.9584	0.0008	
Glycerolipids/ Diradylglycerols/ Diacylglycerols	diacylglycerols	C35H68O5	586.5395	pos/[M+NH4]+	586.5410	0.0015	3.8-3.9
		C36H70O5	600.5556	pos/[M+NH4]+	600.5567	0.0011	
		C37H70O5	612.5561	pos/[M+NH4]+	612.5567	0.0006	
		C37H72O5	614.5701	pos/[M+NH4]+	614.5723	0.0022	
		C38H74O5	628.5873	pos/[M+NH4]+	628.5880	0.0007	
		C39H74O5	640.5874	pos/[M+NH4]+	640.5880	0.0006	
Prenol lipids/ Quinones et hydroquinones/ Ubiquinone	menaquinone	C56H80O2	785.6230	pos/[M+H]+	785.6231	0.0001	3.9
		C56H82O2	787.6314	pos/[M+H]+	787.6388	0.0074	
		C56H80O2	802.6273	pos/[M+NH4]+	802.6491	0.0218	
		C56H82O2	804.6644	pos/[M+NH4]	804.6648	0.0004	
Fatty acyls/ Fatty acyl glycosides/ Fatty acyl glycosides of mono- and disaccharides	glucose monomycolate alpha	C80H154O8	1261.2005	pos/[M+NH4]+	1261.1982	0.0023	4.2
		C82H158O8	1289.2346	pos/[M+NH4]+	1289.2295	0.0051	
		C84H162O8	1317.2636	pos/[M+NH4]+	1317.2608	0.0028	
		C86H166O8	1345.2951	pos/[M+NH4]+	1345.2921	0.0030	
	glucose monomycolate keto	C80H154O9	1277.2276	pos/[M+NH4]+	1277.1931	0.0345	
		C81H156O9	1291.2362	pos/[M+NH4]+	1291.2088	0.0274	
		C83H160O9	1319.2688	pos/[M+NH4]+	1319.2401	0.0287	
		C85H164O9	1347.3013	pos/[M+NH4]+	1347.2714	0.0299	
		C87H168O9	1375.3118	pos/[M+NH4]+	1375.3027	0.0091	
		C88H170O9	1389.3257	pos/[M+NH4]+	1389.3183	0.0074	
		C92H178O9	1445.3766	pos/[M+NH4]+	1445.3809	0.0043	
	glucose monomycolate methoxy	C87H170O9	1377.3118	pos/[M+NH4]+	1377.3183	0.0065	
		C89H174O9	1405.3514	pos/[M+NH4]+	1405.3496	0.0018	
		C91H178O9	1433.3787	pos/[M+NH4]+	1433.3809	0.0022	
		C93H182O9	1461.4119	pos/[M+NH4]+	1461.4122	0.0003	
		C95H186O9	1489.4448	pos/[M+NH4]+	1489.4435	0.0013	
Saccharolipids/ Acyltrehaloses/ Monoacyltrehaloses	trehalose monomycolate alpha	C88H168O13	1451.2845	pos/[M+NH4]+	1451.2823	0.0298	6.2-6.6
		C89H170O13	1465.2817	pos/[M+NH4]+	1465.2980	0.0022	
		C90H172O13	1479.3160	pos/[M+NH4]+	1479.3136	0.0163	
		C91H174O13	1493.3194	pos/[M+NH4]+	1493.3293	0.0290	
		C92H176O13	1507.3476	pos/[M+NH4]+	1507.3449	0.0024	
		C94H180O13	1535.3779	pos/[M+NH4]+	1535.3398	0.0302	
		C96H184O13	1563.4065	pos/[M+NH4]+	1563.3711	0.0118	
	trehalose monomycolate keto	C86H164O14	1439.2757	pos/[M+NH4]+	1439.2459	0.0099	
		C88H168O14	1467.3062	pos/[M+NH4]+	1467.2772	0.0154	
		C89H170O14	1481.3231	pos/[M+NH4]+	1481.2929	0.0027	
		C90H172O14	1495.3239	pos/[M+NH4]+	1495.3065	0.0286	
		C91H174O14	1509.3528	pos/[M+NH4]+	1509.3242	0.0106	
		C92H176O14	1523.3504	pos/[M+NH4]+	1523.3398	0.0106	
		C93H178O14	1537.3818	pos/[M+NH4]+	1537.3555	0.0381	
		C97H186O14	1593.4332	pos/[M+NH4]+	1593.4181	0.0263	
		C99H190O14	1621.4543	pos/[M+NH4]+	1621.4494	0.0021	
		C100H192O14	1635.4611	pos/[M+NH4]+	1635.4650	0.0354	
	trehalose monomycolate methoxy	C89H172O14	1483.3203	pos/[M+NH4]+	1483.3085	0.0031	
		C91H176O14	1511.3504	pos/[M+NH4]+	1511.3398	0.0151	
		C93H180O14	1539.3732	pos/[M+NH4]+	1539.3711	0.0025	
		C95H184O14	1567.4055	pos/[M+NH4]+	1567.4024	0.0008	
		C97H188O14	1595.4382	pos/[M+NH4]+	1595.4337	0.0049	
		C98H190O14	1609.4502	pos/[M+NH4]+	1609.4494	0.0020	
		C99H192O14	1623.4670	pos/[M+NH4]+	1623.4650	0.0039	
		C100H194O14	1637.4842	pos/[M+NH4]+	1637.4807	0.0035	
		C101H196O14	1651.4957	pos/[M+NH4]+	1651.4963	0.0006	
		C102H198O14	1665.5123	pos/[M+NH4]+	1665.5120	0.0003	
		C103H200O14	1679.5254	pos/[M+NH4]+	1679.5276	0.0022	

Saccharolipids/ Acyltrehaloses/ Diacyltrehaloses	diacyltrehalose	C52H96O13	948.7196	pos/[M+NH4]+	948.7715	0.0519	5.7-6.3
		C53H100O13	962.7099	pos/[M+NH4]+	962.7872	0.0773	
		C54H102O13	976.7666	pos/[M+NH4]+	976.7664	0.0002	
		C55H104O13	990.7772	pos/[M+NH4]+	990.7821	0.0049	
		C56H106O13	1004.7908	pos/[M+NH4]+	1004.7977	0.0069	
Polyketide/ Non-ribosomal peptide/ Polyketide hybrids	mycobactins	C46H75O10N5	911.4751	pos/[M+Fe-2H]+	911.4701	0.0050	6.7-6.8
		C47H77O10N5	925.4846	pos/[M+Fe-2H]+	925.4858	0.0012	
		C45H71O10N5	895.4400	pos/[M+Fe-2H]+	895.4388	0.0012	
		C46H73O10N5	909.4576	pos/[M+Fe-2H]+	909.4545	0.0031	
		C47H75O10N5	923.4721	pos/[M+Fe-2H]+	923.4701	0.0020	
Saccharolipids/ Acyltrehaloses/ Acylsulfotrehaloses	tetraacylated sulfoglycolipids	C132H254O20S	2190.8692	neg/[M-H]-	2190.8506	0.0186	6.7-7.2
		C133H256O20S	2204.8851	neg/[M-H]-	2204.8663	0.0188	
		C134H258O20S	2218.8971	neg/[M-H]-	2218.8819	0.0152	
		C135H260O20S	2232.9120	neg/[M-H]-	2232.8976	0.0144	
		C136H262O20S	2246.9298	neg/[M-H]-	2246.9132	0.0166	
		C137H264O20S	2260.9434	neg/[M-H]-	2260.9289	0.0145	
		C138H266O20S	2274.9565	neg/[M-H]-	2274.9445	0.0120	
		C139H268O20S	2288.9711	neg/[M-H]-	2288.9602	0.0109	
		C140H270O20S	2302.9906	neg/[M-H]-	2302.9758	0.0148	
		C139H268O21S	2304.9870	neg/[M-H]-	2304.9551	0.0319	
		C141H272O20S	2317.0025	neg/[M-H]-	2316.9915	0.0110	
		C140H270O21S	2319.0011	neg/[M-H]-	2318.9708	0.0303	
		C142H274O20S	2331.0132	neg/[M-H]-	2331.0071	0.0061	
Saccharolipids/ Acyltrehaloses/ Acylsulfotrehaloses	tetraacylated sulfoglycolipids (continued)	C141H272O21S	2333.0122	neg/[M-H]-	2332.9864	0.0258	6.7-7.2
		C143H276O20S	2345.0285	neg/[M-H]-	2345.0228	0.0057	
		C142H274O21S	2347.0308	neg/[M-H]-	2347.0021	0.0287	
		C144H278O20S	2359.0448	neg/[M-H]-	2359.0384	0.0064	
		C143H276O21S	2361.0459	neg/[M-H]-	2361.0177	0.0282	
		C144H278O21S	2373.0549	neg/[M-H]-	2373.0177	0.0372	
		C146H282O20S	2387.0705	neg/[M-H]-	2387.0697	0.0008	
		C145H280O21S	2389.0727	neg/[M-H]-	2389.0490	0.0237	
		C147H284O20S	2401.0860	neg/[M-H]-	2401.0854	0.0006	
		C146H282O21S	2403.0891	neg/[M-H]-	2403.0647	0.0244	
		C148H286O20S	2415.0943	neg/[M-H]-	2415.1010	0.0067	
		C147H284O21S	2417.1044	neg/[M-H]-	2417.0803	0.0241	
		C149H288O20S	2429.1047	neg/[M-H]-	2429.1167	0.0120	
		C148H286O21S	2431.1160	neg/[M-H]-	2431.0960	0.0200	
		C150H290O20S	2443.1274	neg/[M-H]-	2443.1323	0.0049	
		C149H288O21S	2445.1329	neg/[M-H]-	2445.1116	0.0213	
		C151H292O20S	2457.1311	neg/[M-H]-	2457.1480	0.0169	
		C150H290O21S	2459.1460	neg/[M-H]-	2459.1273	0.0187	
		C152H294O20S	2471.1445	neg/[M-H]-	2471.1636	0.0191	
		C151H292O21S	2473.1626	neg/[M-H]-	2473.1429	0.0197	
		C152H292O21S	2485.1598	neg/[M-H]-	2485.1429	0.0169	
		C152H294O21S	2487.1783	neg/[M-H]-	2487.1586	0.0197	
		C153H294O21S	2499.1729	neg/[M-H]-	2499.1586	0.0143	
		C153H296O21S	2501.1936	neg/[M-H]-	2501.1742	0.0194	
		C154H296O21S	2513.1795	neg/[M-H]-	2513.1742	0.0053	
		C154H298O21S	2515.2066	neg/[M-H]-	2515.1899	0.0167	
		C155H298O21S	2527.1964	neg/[M-H]-	2527.1899	0.0065	
		C155H300O21S	2529.2214	neg/[M-H]-	2529.2055	0.0159	
		C156H300O21S	2541.2173	neg/[M-H]-	2541.2055	0.0118	
		C156H302O21S	2543.2374	neg/[M-H]-	2543.2212	0.0162	
		C157H302O21S	2555.2211	neg/[M-H]-	2555.2212	0.0001	
		C157H304O21S	2557.2514	neg/[M-H]-	2557.2368	0.0146	
		C158H304O21S	2569.2344	neg/[M-H]-	2569.2368	0.0024	
		C158H306O21S	2571.2632	neg/[M-H]-	2571.2525	0.0107	
		C159H306O21S	2583.2484	neg/[M-H]-	2583.2525	0.0041	
		C159H308O21S	2585.2762	neg/[M-H]-	2585.2681	0.0101	
		C160H308O21S	2597.2599	neg/[M-H]-	2597.2681	0.0082	
		C160H310O21S	2599.2924	neg/[M-H]-	2599.2838	0.0086	
		C161H312O21S	2613.3004	neg/[M-H]-	2613.2994	0.0010	
		C162H312O21S	2625.2944	neg/[M-H]-	2625.2994	0.0050	
		C162H314O21S	2627.3244	neg/[M-H]-	2627.3151	0.0093	
		C163H316O21S	2641.3358	neg/[M-H]-	2641.3307	0.0051	
		C164H318O21S	2655.3514	neg/[M-H]-	2655.3464	0.0050	
		C165H320O21S	2669.3710	neg/[M-H]-	2669.3620	0.0090	
		C166H322O21S	2683.3866	neg/[M-H]-	2683.3777	0.0089	
		C167H324O21S	2697.3967	neg/[M-H]-	2697.3933	0.0054	
		C168H326O21S	2711.4129	neg/[M-H]-	2711.4090	0.0039	
		C169H328O21S	2725.4339	neg/[M-H]-	2725.4246	0.0093	
		C170H330O21S	2739.4366	neg/[M-H]-	2739.4403	0.0037	
		C171H332O21S	2753.4551	neg/[M-H]-	2753.4559	0.0008	
		C172H334O21S	2767.4443	neg/[M-H]-	2767.4716	0.0273	
		C173H336O21S	2781.4768	neg/[M-H]-	2781.4872	0.0104	

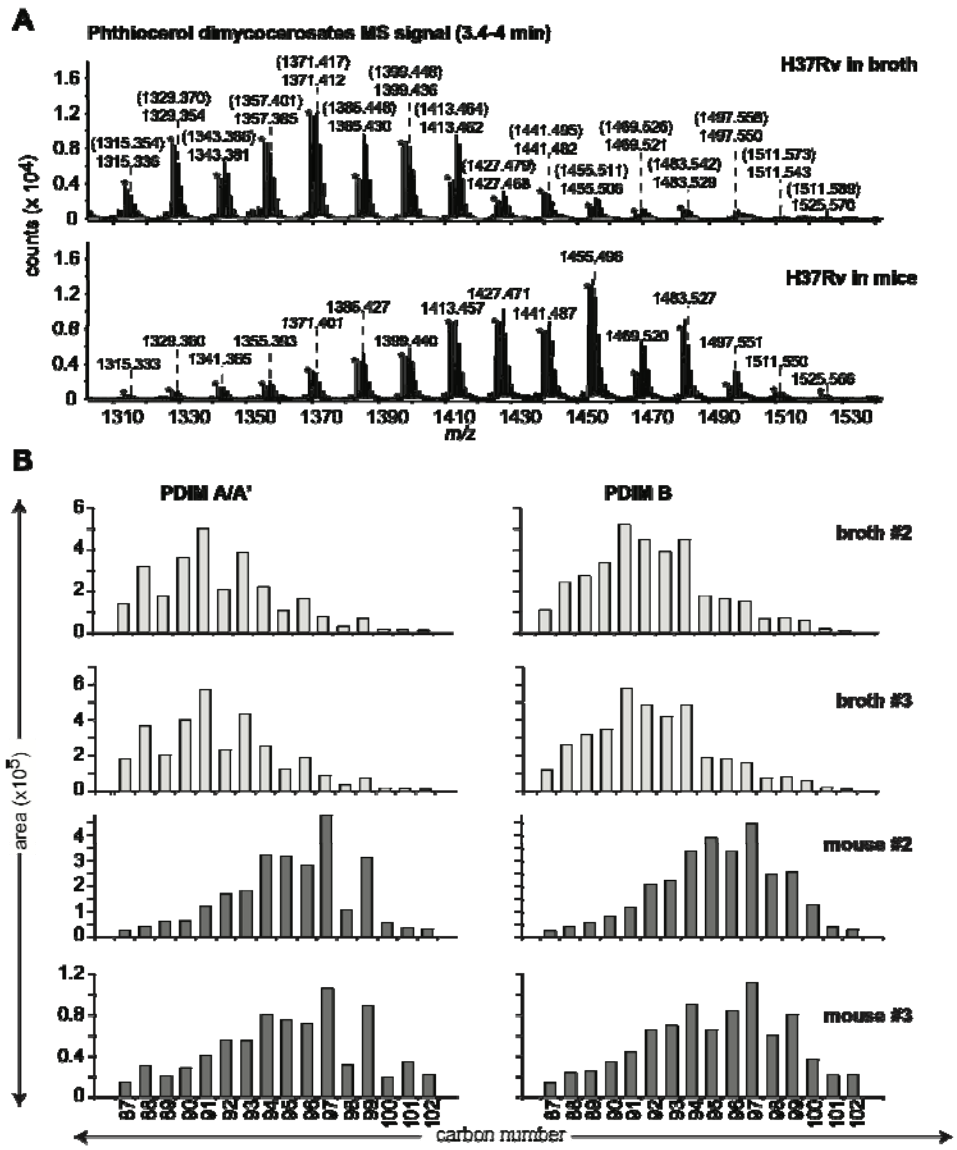


Figure S6, related to Figure 5. Mapping the *in vitro* and *in vivo* phthiocerol dimycocerosate (PDIM) alkylforms of *M. tuberculosis.* (**A**) Positive-ion mode spectra of PDIM observed by analyzing the lipidic extract of *M. tuberculosis* Erdman 2.5 grown in broth culture or mice infection experiments, which shows marked increases in the overall size of the PDIM series. Detected *m/z* of the $[M+NH_4]^+$ adducts of PDIM A/A' are indicated. Calculated *m/z* of the respective ions are indicated in parentheses. PDIM B species are also detected and labeled with stars. (**B**) Areas of extracted ion chromatograms of individual PDIM A/A' andB alkylforms (97 to 102 total carbons) detected for 2 independent broth cultures of *M. tuberculosis* Erdman and for lipidic extracts obtained from homogenized lungs of 2 infected mice. Results show a lengthening of PDIM alkylforms during mice infection, which are replicate experiments of that presented in **Figure 5**.

A

M	Adduct	Median detected m/z	Isotopes	Median RT (min)	p-value	Absolute fold change
1785.473	Na	1808.450	M	4.08	1.34E-04	28982.57
		1809.454	M+1	4.16	3.42E-05	40984.27
1813.505	NH_4	1831.540	M	3.79	1.83E-05	17958.11
		1832.543	M+1	3.77	2.65E-03	18462.91
	Na	1836.483	M	4.07	2.72E-05	62642.93
		1837.485	M+1	4.07	6.64E-06	74851.41
		1838.478	M+2	4.06	8.96E-05	32467.20
1825.505	NH_4	1844.556	M+1	3.76	3.68E-06	8839.25
1827.520	NH_4	1845.535	M	3.94	1.09E-05	43648.46
		1846.551	M+1	3.81	1.81E-04	33096.34
		1847.575	M+2	3.77	2.54E-05	12809.09
	Na	1850.486	M	4.05	6.60E-04	64466.20
		1851.499	M+1	4.04	2.00E-05	73895.10
		1852.485	M+2	4.05	2.72E-05	52512.88
1841.536	NH_4	1859.567	M	3.85	1.81E-05	27980.25
		1860.536	M+1	4.02	5.13E-05	38034.63
		1861.570	M+2	3.81	1.81E-05	13016.09
	Na	1864.510	M	4.02	1.34E-04	46000.47
		1865.503	M+1	4.06	2.66E-05	54686.07
		1866.506	M+2	4.09	3.61E-06	37001.08

M	Adduct	Median detected m/z	Isotopes	Median RT (min)	p-value	Absolute fold change
1853.536	Na	1876.564	M	3.80	1.81E-05	13638.51
1855.552	NH_4	1874.564	M+1	3.93	2.64E-04	48097.83
		1875.564	M+2	3.79	1.81E-05	26158.62
	Na	1878.525	M	4.04	1.81E-05	62423.84
		1879.531	M+1	4.04	3.90E-05	66939.63
		1880.524	M+2	4.04	1.83E-05	43589.66
1869.567	NH_4	1887.592	M	3.79	2.78E-03	64.93
		1888.578	M+1	4.01	4.85E-05	70469.32
		1889.596	M+2	3.78	6.53E-03	50.78
	Na	1892.523	M	4.03	1.81E-05	74169.84
		1893.537	M+1	4.03	4.15E-05	71845.32
		1894.532	M+2	4.02	3.35E-04	32183.20
1883.583	NH_4	1901.607	M	3.82	3.53E-05	11309.09
		1902.610	M+1	3.78	2.04E-05	14230.87
	Na	1906.569	M	3.70	2.72E-05	9007.25
1897.599	NH_4	1915.627	M	3.75	5.80E-05	7798.98
		1916.632	M+1	3.76	7.44E-05	7323.43
1911.614	NH_4	1930.645	M+1	3.74	1.03E-06	13151.86

B **Structure and MS signal (3.7-4.2 min) of triglycosylated phenolic glycolipids**

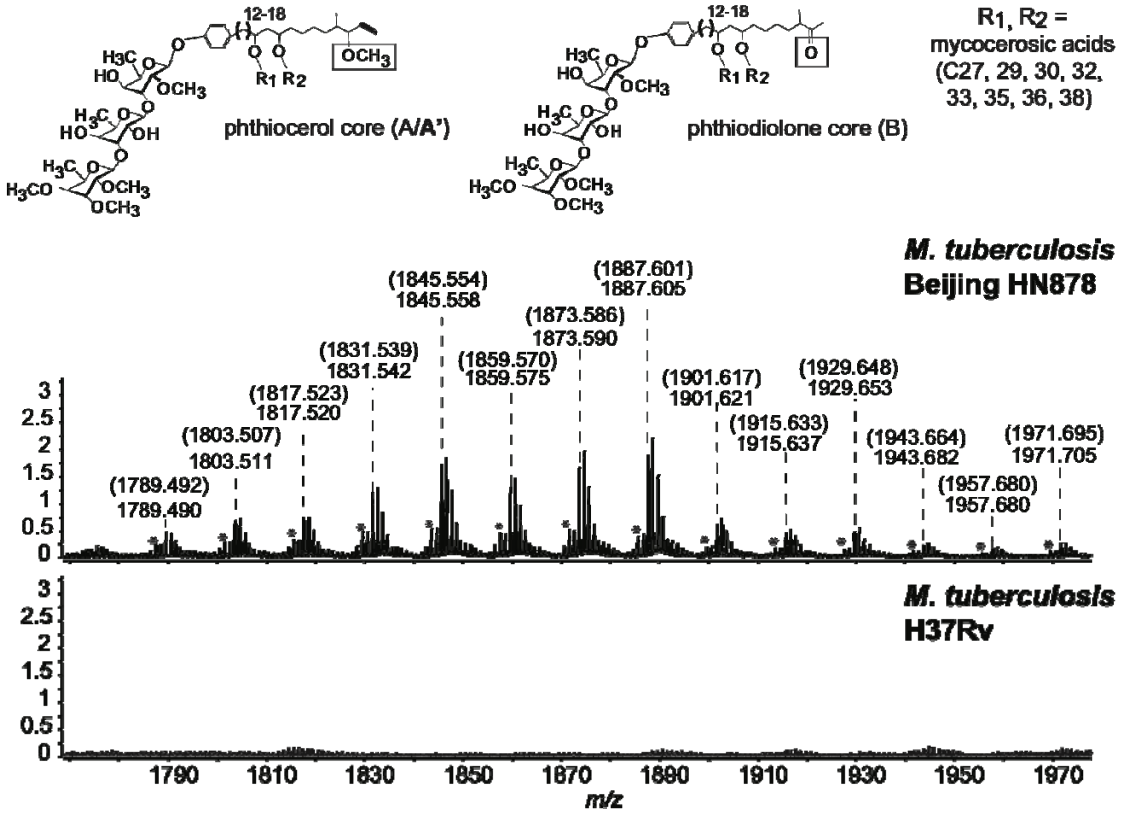


Figure S7, related to Figure 6. Chemotaxonomy of the virulent *M. tuberculosis* Beijing strains. (**A**) Among the features identified by Mass Profiler Professional as over-represented in *M. tuberculosis* Beijing dataset, 38 correspond to alternate adducts and isotopesof the PGL as shown in **Figure 6**. Specifically, the features correspond to ammonium or sodium adducts of 10 members of the PGL alkane series with similar retention times. Fold change and p-value calculated by Mass Profiler Pro are reported for each feature. (**B**) Structure and MS signal of triglycosylated phenolic glycolipids (PGL) composed of phenolphthiocerol core (A/**A'**), in which the bold letter designates an additional methylene for the A' subclass, or composed of phenolphthiodiolone core for the B subclass (B). MS signal of the PGL A/A' and B detected by analyzing the lipidic extract of *M. tuberculosis* Beijing (top) and MS signal extracted at the same retention for the parallel analysis of the lipidic extract of *M. tuberculosis* H37Rv (bottom). Detected *m/z* of the $[M+NH_4]^+$ adducts of PGL A/A' are indicated. Calculated *m/z* of the respective ions are indicated in parentheses. $[M+NH_4]^+$ adducts of PGL B are also detected and labeled by stars.

SUPPLEMENTAL EXPERIMENTAL PROCEDURES

The MycoMass database

To compile the *MycoMass* database, the following articles have been used for providing updated lipid structures (sorted by lipid family alphabetic order). Acyl trehaloses: diacylated (Ariza and Valero-Guillen, 1994; Lemassu et al., 1991), triacylated (Minnikin et al., 2002), polyacylated (Daffe et al., 1988), mycobactins and carboxymycobactins (Madigan C.A. et al, submitted), cardiolipin (Hsu and Turk, 2006), carotenes (Robledo et al., 2011), decaprenylphosphoribose (Huang et al., 2005), diglycosylated diacylglycerol (Hunter et al., 1986), exochelins (Gobin et al., 1999; Ratledge, 2004), fatty acids (Walker et al., 1970), glucose monomycolates (Laval et al., 2008), glucuronosyl diacylglycerol (Wolucka et al., 1993), glycerides: triacylated (Walker et al., 1970), monomeromycolyl-diacylated (Burguiere et al., 2005), glycerol monomycolates (Layre et al., 2009), glycopeptidolipids (Bozic et al., 1988; Chatterjee and Khoo, 2001; Kano et al., 2005; Miyamoto et al., 2006; Villeneuve et al., 2003), hydroxybenzoic acid derivatives (Constant et al., 2002), leprosol (Bu'Lock and Hudson, 1969), lipooligosaccharides (Burguiere et al., 2005), lipopentapeptides (Biet et al., 2008), menaquinone (Dhiman et al., 2009; Dunphy et al., 1971), sulfated menaquinone (Holsclaw et al., 2008), mycoketides (Matsunaga et al., 2004), mycolactone (Hong et al., 2008), mycolic acids (Laval et al., 2001), mycolipanolic acid, mycolipodienic acid, mycosanoic acids, mycocerosic acids and phthienoic acids (Rousseau et al., 2003; Sirakova et al., 2001), mycothiol (Newton et al., 2008), phospholipids (Gilleron et al., 2006; Walker et al., 1970), phosphatidylethanolamine lysinilated (Maloney et al., 2009), phosphatidylinositol mannosides (Gilleron et al., 2006; Gilleron et al., 2003), phenolic glycolipids: A/B (Constant et al., 2002), B1, B2, B3 (Vercellone and Puzo, 1989), phthiotriol and C16phthiotriol (Huet et al., 2009), phthiocerol dimycocerosates (Camacho et al., 2001; Constant et al., 2002; Huet et al., 2009), sulfoglycolipids, phthioceric acids, hydroxyphthioceranic acid (Layre et al., 2011), trehalose dimycolates (Kai et al., 2007), trehalose monomycolates (Fujita et al., 2005; Laval et al., 2001).

R script for automated annotation of features

We designed a script written in R langage for automatic annotation of feature list exported as a .csv file. The following script is used for the annotation of features aquired in positive-ion mode and that match any *MycoMass* entry within 10ppm.

```
annotate.ion.finding <- function(masses.file, db.file, ppmthresh, rtthresh, out.file) {
  massesin <- read.csv(masses.file, header = TRUE)
  masses <- massesin[,1]
  lipids <- read.csv(db.file, header = FALSE, quote="\"", as.is = TRUE, skip=5)
  lipid.names <- paste(lipids[,6],"(",lipids[,7],":",lipids[,8],")", sep = "")
  h <- as.double(lipids[,16])
  nh4 <- as.double(lipids[,17])
  na <- as.double(lipids[,18])
  fe3 <- as.double(lipids[,19])
  lipid.names.updated <- array(0, length(lipid.names))
  lipid.masses <- array(0, length(lipid.names))

  for (i in 1:length(lipid.names)){
   lipid.names.updated[4*i-3]<- paste(lipid.names[i],"H+",sep="")
   lipid.masses[4*i-3] <- h[i]
   lipid.names.updated[4*i-2]<- paste(lipid.names[i],"NH4+",sep="")
   lipid.masses[4*i-2] <- nh4[i]
   lipid.names.updated[4*i-1]<- paste(lipid.names[i],"Na+",sep="")
   lipid.masses[4*i-1] <- na[i]
   lipid.names.updated[4*i]<- paste(lipid.names[i],"Fe3+-2H",sep="")
   lipid.masses[4*i] <- fe3[i]
}
  hit <- list()
  for (i in 1:length(masses)) {
    hit[[i]] <- na.omit(lipid.names.updated[abs(lipid.masses-
masses[i])/lipid.masses*1000000<ppmthresh])
}
  maxcol <- max(sapply(hit,length))
  names <- matrix(" ", ncol=maxcol, nrow=length(masses))
  for (i in 1:nrow(names)) {
    names[i, ] <- c(hit[[i]], rep(" ", maxcol - length(hit[[i]])))
    if (names[i,1] == " "){names[i,1] <- "No Hit"}
}
  names
  write.table(names, file=out.file, quote=FALSE,row.names=FALSE, col.names=FALSE)
  return(names)
}
db.file="Figure_S1_MycoMass_database.csv"
```

```
masses.file="XCMS_Output.csv"
out.file="Annotation_Results_Positive.txt"
names<-annotate.ion.finding(masses.file, db.file, ppmthresh=10, rtthresh=1000, out.file)
```

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